Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 10:58 AM GMT

PDB ID	:	3NM1
Title	:	The Crystal Structure of Candida glabrata THI6, a Bifunctional Enzyme involved in Thiamin Biosyhthesis of Eukaryotes
Authors	:	Paul, D.; Chatterjee, A.; Begley, T.P.; Ealick, S.E.
Deposited on	:	2010-06-21
Resolution	:	3.21 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

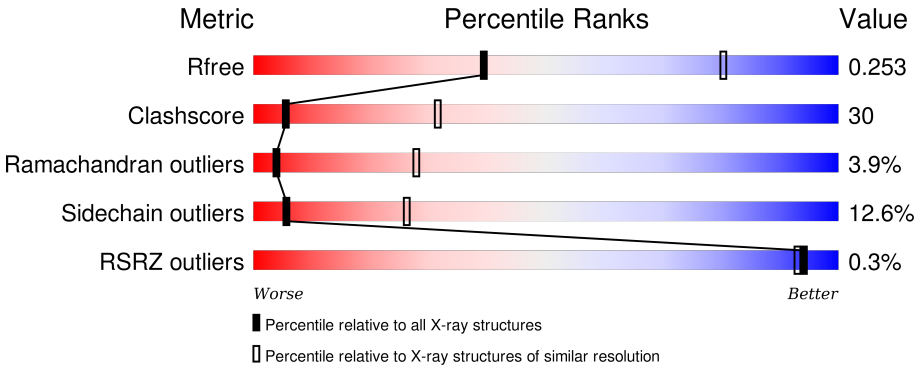
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.21 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1095 (3.26-3.18)
Clashscore	102246	1046 (3.24-3.20)
Ramachandran outliers	100387	1026 (3.24-3.20)
Sidechain outliers	100360	1025 (3.24-3.20)
RSRZ outliers	91569	1100 (3.26-3.18)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	540	47% 40% 6% 6%
1	B	540	47% 40% 6% • 6%
1	C	540	% 46% 40% 7% • 6%
1	D	540	50% 36% 7% • 6%
1	E	540	49% 36% 8% • 6%

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Mol	Chain	Length	Quality of chain
1	F	540	49% 38% 6% 6%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	MG	A	544	-	-	-	X
5	MG	D	544	-	-	-	X
5	MG	E	544	-	-	-	X

2 Entry composition

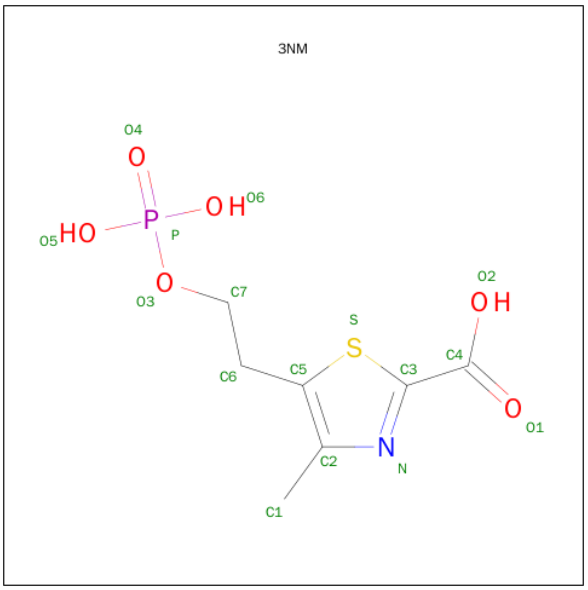
There are 5 unique types of molecules in this entry. The entry contains 22801 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Thiamine biosynthetic bifunctional enzyme.

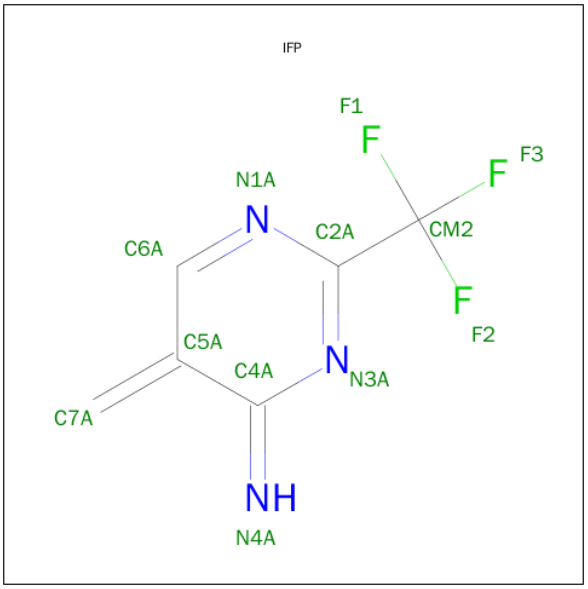
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	507	Total	C	N	O	S	0	0	0
			3765	2386	632	726	21			
1	B	507	Total	C	N	O	S	0	0	0
			3765	2386	632	726	21			
1	C	507	Total	C	N	O	S	0	0	0
			3765	2386	632	726	21			
1	D	507	Total	C	N	O	S	0	0	0
			3765	2386	632	726	21			
1	E	505	Total	C	N	O	S	0	0	0
			3748	2375	629	723	21			
1	F	507	Total	C	N	O	S	0	0	0
			3765	2386	632	726	21			

- Molecule 2 is 4-METHYL-5-[2-(PHOSPHONOOXY)ETHYL]-1,3-THIAZOLE-2-CARBOXYLIC ACID (three-letter code: 3NM) (formula: $C_7H_{10}NO_6PS$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			16	7	1	6	1	1		
2	F	1	Total	C	N	O	P	S	0	0
			16	7	1	6	1	1		
2	E	1	Total	C	N	O	P	S	0	0
			16	7	1	6	1	1		
2	D	1	Total	C	N	O	P	S	0	0
			16	7	1	6	1	1		
2	C	1	Total	C	N	O	P	S	0	0
			16	7	1	6	1	1		
2	B	1	Total	C	N	O	P	S	0	0
			16	7	1	6	1	1		

- Molecule 3 is 2-TRIFLUOROMETHYL-5-METHYLENE-5H-PYRIMIDIN-4-YLIDENEAMINE (three-letter code: IFP) (formula: $C_6H_4F_3N_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	F	N	0	0
			12	6	3	3		
3	F	1	Total	C	F	N	0	0
			12	6	3	3		
3	E	1	Total	C	F	N	0	0
			12	6	3	3		
3	D	1	Total	C	F	N	0	0
			12	6	3	3		
3	C	1	Total	C	F	N	0	0
			12	6	3	3		

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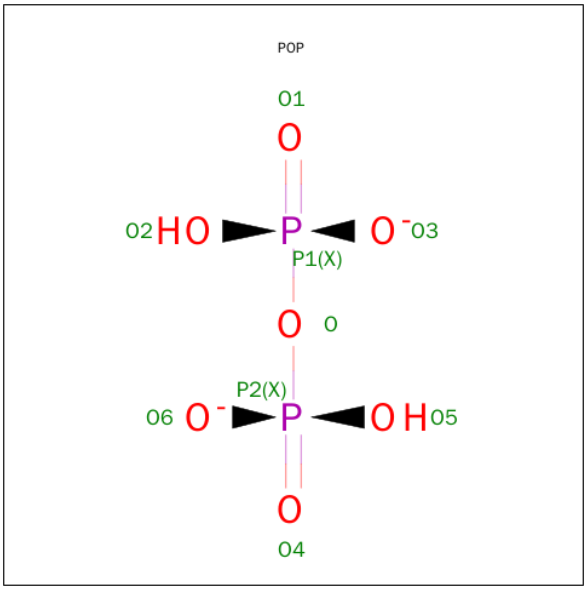
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C F N 12 6 3 3	0	0

- Molecule 4 is PYROPHOSPHATE 2- (three-letter code: POP) (formula: $H_2O_7P_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O P 9 7 2	0	0
4	F	1	Total O P 9 7 2	0	0
4	E	1	Total O P 9 7 2	0	0
4	D	1	Total O P 9 7 2	0	0
4	C	1	Total O P 9 7 2	0	0
4	B	1	Total O P 9 7 2	0	0

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	1	Total Mg 1 1	0	0
5	E	1	Total Mg 1 1	0	0

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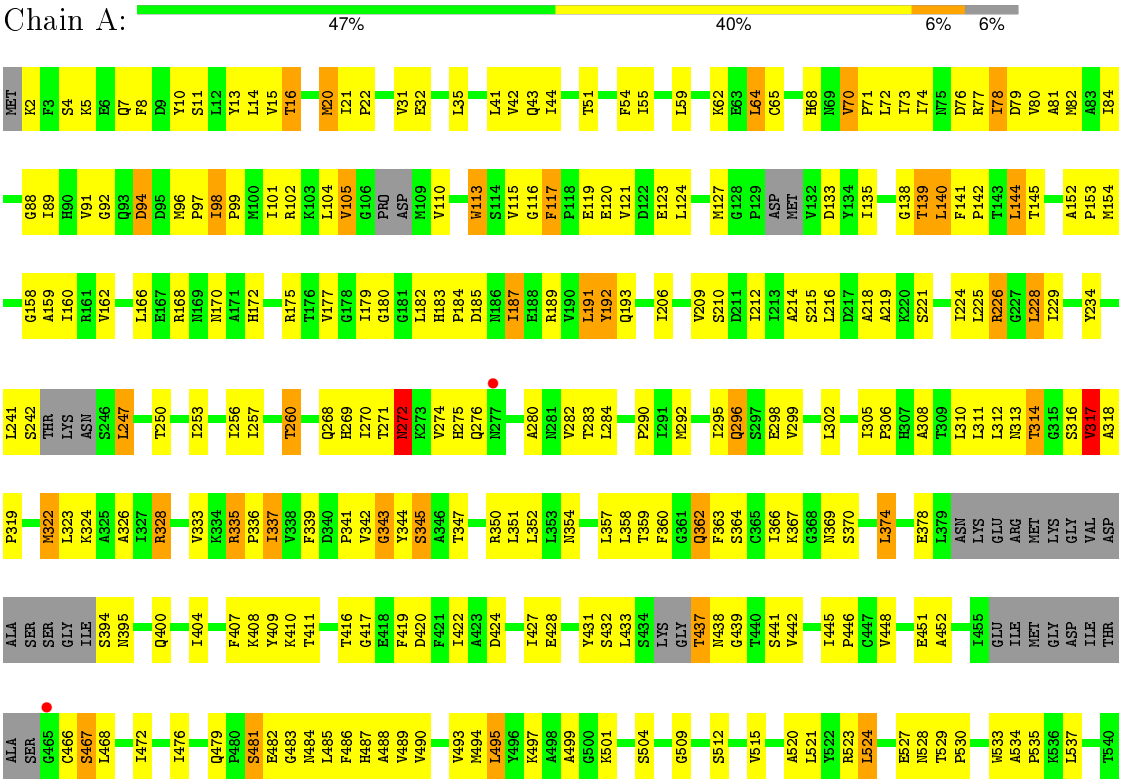
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total Mg 1 1	0	0
5	C	1	Total Mg 1 1	0	0
5	A	1	Total Mg 1 1	0	0
5	F	1	Total Mg 1 1	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

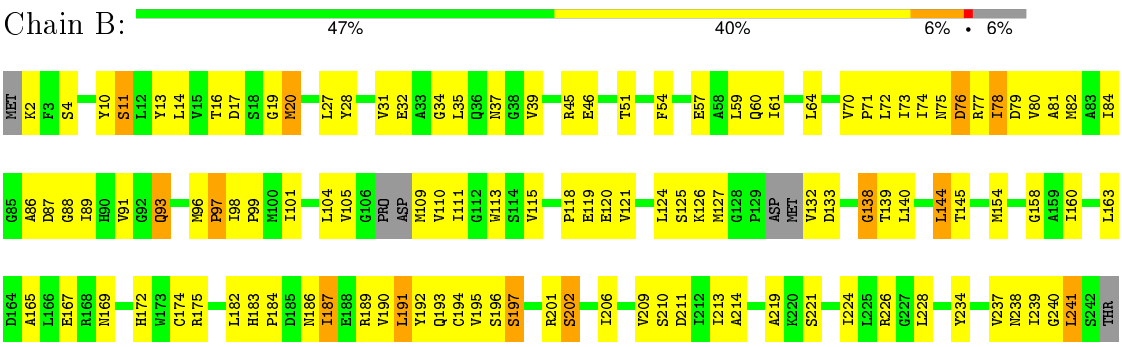
- Molecule 1: Thiamine biosynthetic bifunctional enzyme

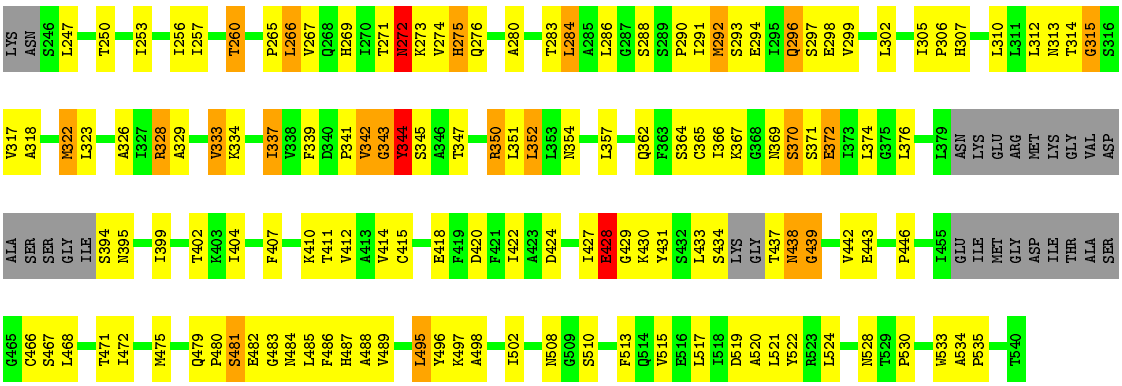
Chain A:



- Molecule 1: Thiamine biosynthetic bifunctional enzyme

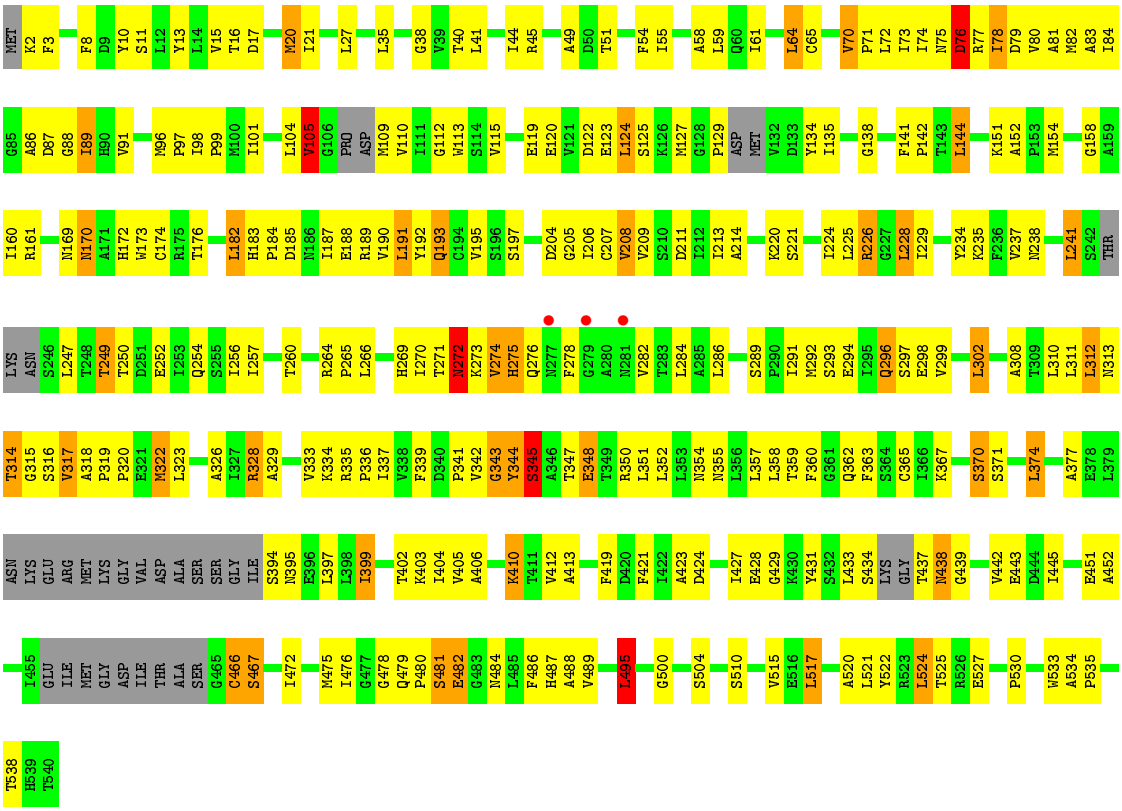
Chain B:





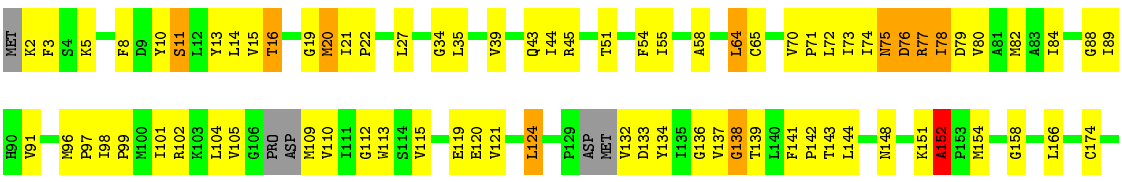
• Molecule 1: Thiamine biosynthetic bifunctional enzyme

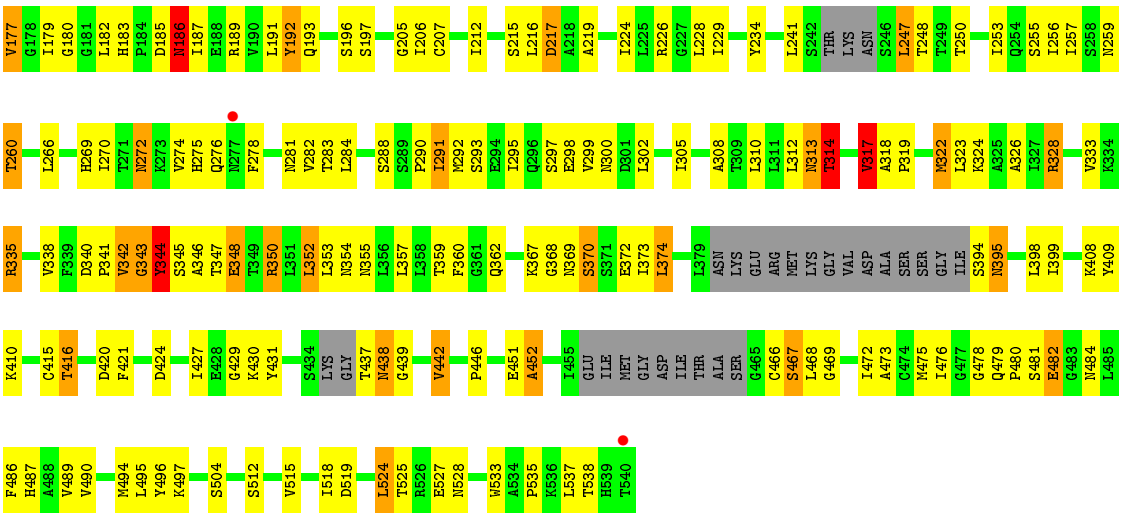
Chain C:



• Molecule 1: Thiamine biosynthetic bifunctional enzyme

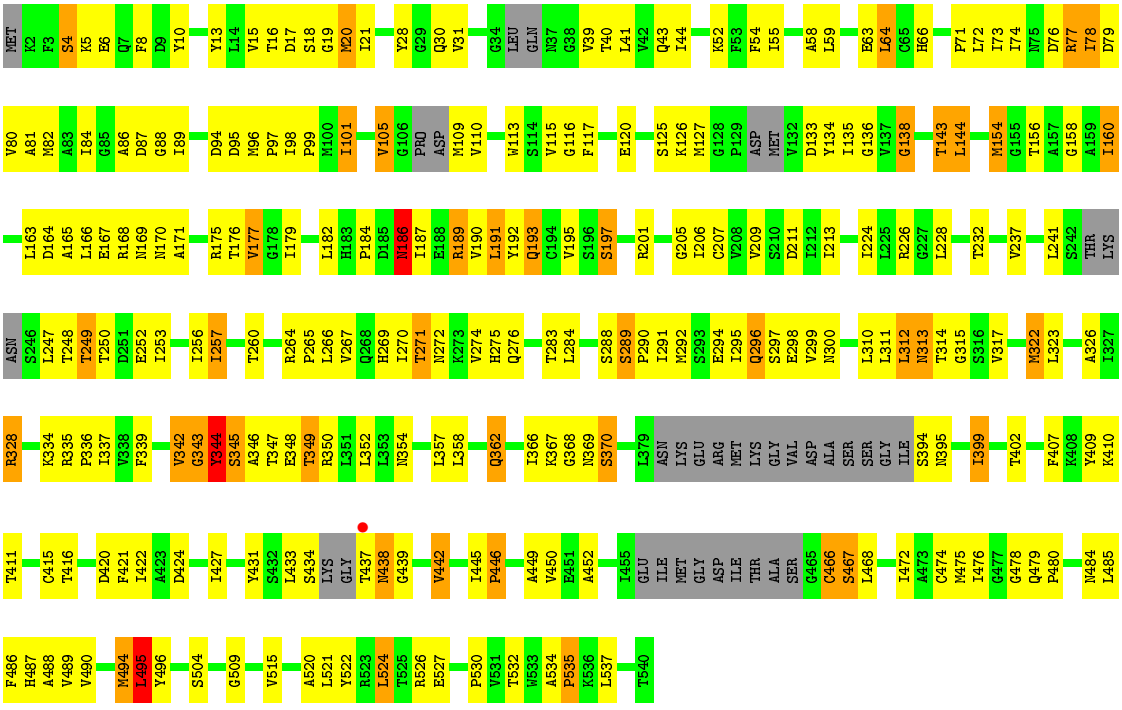
Chain D:





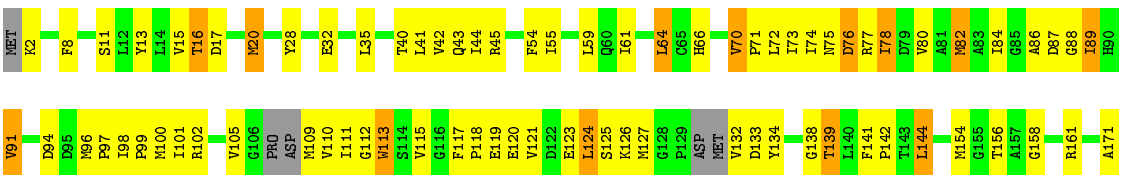
• Molecule 1: Thiamine biosynthetic bifunctional enzyme

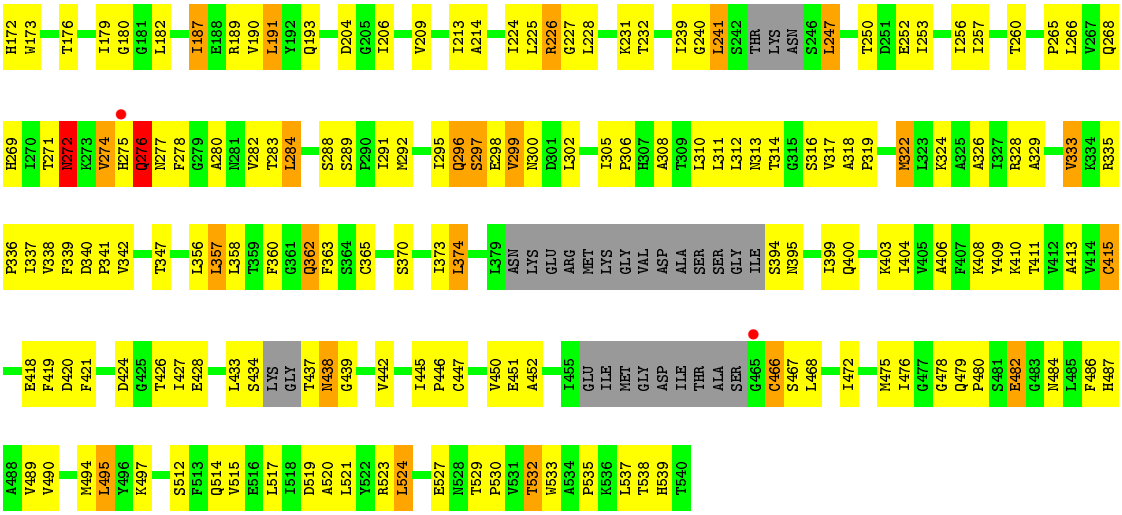
Chain E:



• Molecule 1: Thiamine biosynthetic bifunctional enzyme

Chain F:




H172 W173 T176 I179 G180 G181 L182 I187 E188 R189 V190 L191 Y192 Q193 D204 G205 I206 V209 I213 A214 I224 L225 R226 G227 L228 K231 T232 I239 G240 L241 S242 THR LYS ASN S246 L247 T250 D251 E252 I253 I256 I257 T260 P265 L266 V267 Q268
H269 I270 T271 N272 K273 V274 H275 Q276 N277 F278 G279 A280 N281 V282 T283 L284 S288 S289 P290 I291 M292 I295 Q296 S297 E298 V299 N300 D301 L302 I305 P306 H307 A308 T309 L310 L311 L312 N313 T314 G315 S316 V317 A318 P319 M322 L323 K324 A325 A326 I327 R328 A329 V333 K334 R335
P336 I337 V338 F339 D340 P341 V342 T347 L356 L357 L358 T359 F360 G361 Q362 F363 S364 C365 S370 I373 L374 L379 ASN LYS GLU ARG MET LYS GLY VAL ASP ALA SER SER GLY ILE S394 N395 I399 Q400 K403 I404 V405 A406 F407 K408 Y409 K410 T411 V412 A413 V414 C415
E418 F419 D420 F421 D424 G425 T426 I427 E428 L433 S434 LYS GLY T437 N438 G439 V442 I445 P446 C447 V450 E451 A452 I455 GLU ILE MET GLY ASP ILE THR ALA SER G465 C466 S467 L468 I472 M475 I476 G477 G478 Q479 P480 S481 E482 G483 N484 L485 F486 H487
A488 V489 V490 M494 L495 Y496 K497 S512 F513 Q514 V515 E516 L517 T518 D519 A520 L521 Y522 R523 L524 E527 N528 T529 P530 V531 T532 W533 A534 P535 K536 L537 T538 H539 T540

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	104.94Å 154.21Å 148.70Å 90.00° 102.10° 90.00°	Depositor
Resolution (Å)	38.55 – 3.21 38.55 – 3.21	Depositor EDS
% Data completeness (in resolution range)	97.8 (38.55-3.21) 97.9 (38.55-3.21)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	6.65 (at 3.18Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor
R, R_{free}	0.201 , 0.232 0.197 , 0.253	Depositor DCC
R_{free} test set	3731 reflections (5.31%)	DCC
Wilson B-factor (Å^2)	72.8	Xtriage
Anisotropy	0.553	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 49.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 73983 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	22801	wwPDB-VP
Average B, all atoms (Å^2)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.82% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 3NM, IFP, POP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.48	0/3824	0.70	2/5190 (0.0%)
1	B	0.46	0/3824	0.67	2/5190 (0.0%)
1	C	0.49	0/3824	0.70	3/5190 (0.1%)
1	D	0.50	0/3824	0.74	4/5190 (0.1%)
1	E	0.48	0/3806	0.70	2/5164 (0.0%)
1	F	0.47	0/3824	0.65	0/5190
All	All	0.48	0/22926	0.69	13/31114 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	1	0
1	D	0	1
All	All	1	1

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	317	VAL	CB-CA-C	-15.99	81.02	111.40
1	C	345	SER	N-CA-CB	-13.34	90.49	110.50
1	A	345	SER	N-CA-CB	-12.85	91.22	110.50
1	E	345	SER	N-CA-CB	-12.75	91.38	110.50
1	E	344	TYR	CB-CA-C	12.68	135.76	110.40
1	C	344	TYR	CB-CA-C	12.31	135.03	110.40
1	B	345	SER	N-CA-CB	-12.21	92.19	110.50
1	A	344	TYR	CB-CA-C	11.09	132.58	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	344	TYR	CB-CA-C	10.65	131.69	110.40
1	D	344	TYR	CB-CA-C	10.58	131.56	110.40
1	D	345	SER	N-CA-CB	-8.33	98.00	110.50
1	D	152	ALA	CB-CA-C	5.17	117.85	110.10
1	C	76	ASP	N-CA-C	5.02	124.55	111.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	344	TYR	CA

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	317	VAL	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3765	0	3750	262	0
1	B	3765	0	3750	230	0
1	C	3765	0	3750	221	0
1	D	3765	0	3750	218	0
1	E	3748	0	3730	223	0
1	F	3765	0	3750	226	0
2	A	16	0	7	3	0
2	B	16	0	7	3	0
2	C	16	0	7	0	0
2	D	16	0	7	1	0
2	E	16	0	7	2	0
2	F	16	0	7	2	0
3	A	12	0	4	1	0
3	B	12	0	4	1	0
3	C	12	0	4	0	0
3	D	12	0	4	0	0
3	E	12	0	4	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	12	0	4	0	0
4	A	9	0	0	1	0
4	B	9	0	0	2	0
4	C	9	0	0	0	0
4	D	9	0	0	0	0
4	E	9	0	0	0	0
4	F	9	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
All	All	22801	0	22546	1342	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 30.

All (1342) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:78:ILE:HG21	1:B:96:MET:HE1	1.33	1.10
1:F:78:ILE:HG21	1:F:96:MET:HE1	1.34	1.09
1:B:343:GLY:HA3	1:B:350:ARG:HD3	1.29	1.09
1:F:8:PHE:CE2	1:F:110:VAL:HG21	1.91	1.06
1:A:313:ASN:ND2	1:A:342:VAL:HG21	1.71	1.06
1:E:77:ARG:HG2	1:E:77:ARG:HH11	1.18	1.04
1:D:317:VAL:O	1:D:317:VAL:CG1	1.91	1.03
1:D:299:VAL:HG21	1:D:326:ALA:HA	1.40	1.03
1:C:96:MET:HE3	1:C:101:ILE:HG12	1.37	1.03
1:D:317:VAL:HG12	1:D:317:VAL:O	1.19	1.01
1:A:78:ILE:HG21	1:A:96:MET:HE1	1.43	0.99
1:B:366:ILE:HD12	1:B:411:THR:HG21	1.43	0.99
1:A:187:ILE:HG12	1:A:206:ILE:HD13	1.41	0.99
1:D:77:ARG:HG2	1:D:77:ARG:HH11	1.26	0.97
1:C:274:VAL:HG23	1:C:275:HIS:HD2	1.25	0.96
1:C:299:VAL:HG21	1:C:326:ALA:HA	1.48	0.96
1:A:8:PHE:CE2	1:A:110:VAL:HG11	2.00	0.95
1:A:313:ASN:HD21	1:A:342:VAL:HG21	1.31	0.95
1:C:343:GLY:HA3	1:C:350:ARG:HD3	1.47	0.93
1:A:343:GLY:HA3	1:A:350:ARG:HD3	1.49	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:314:THR:HG21	1:E:354:ASN:HD21	1.34	0.93
1:C:144:LEU:HD12	1:C:144:LEU:H	1.33	0.92
1:A:154:MET:HG2	1:A:158:GLY:HA3	1.51	0.91
1:B:115:VAL:HG13	1:B:120:GLU:HB2	1.53	0.91
1:E:366:ILE:HD12	1:E:411:THR:HG21	1.50	0.90
1:B:484:ASN:ND2	1:B:487:HIS:H	1.69	0.90
1:C:78:ILE:HG21	1:C:96:MET:CE	2.01	0.89
1:A:339:PHE:CE2	1:A:341:PRO:HG3	2.07	0.89
1:E:110:VAL:HG23	1:E:133:ASP:HB2	1.55	0.88
1:A:299:VAL:HG21	1:A:326:ALA:HA	1.55	0.88
1:F:250:THR:HG23	1:F:530:PRO:HB2	1.55	0.88
1:F:8:PHE:HE2	1:F:110:VAL:HG21	1.37	0.88
1:D:192:TYR:HD1	1:D:234:TYR:HD2	1.20	0.88
1:E:299:VAL:HG21	1:E:326:ALA:HA	1.54	0.88
1:D:276:GLN:HG3	1:D:292:MET:HE2	1.57	0.87
1:F:339:PHE:CE2	1:F:341:PRO:HG3	2.10	0.87
1:A:367:LYS:NZ	1:A:466:CYS:HA	1.88	0.87
1:D:187:ILE:HG12	1:D:206:ILE:HD13	1.58	0.86
1:D:183:HIS:H	1:D:186:ASN:HD21	1.19	0.86
1:F:78:ILE:HG21	1:F:96:MET:CE	2.06	0.85
1:E:343:GLY:HA3	1:E:350:ARG:HD3	1.58	0.85
1:E:101:ILE:O	1:E:105:VAL:HG22	1.76	0.85
1:A:35:LEU:HD22	1:A:70:VAL:HG11	1.59	0.85
1:A:313:ASN:ND2	1:A:342:VAL:CG2	2.39	0.85
1:B:35:LEU:HD21	1:B:70:VAL:HG11	1.59	0.85
1:C:274:VAL:HG23	1:C:275:HIS:CD2	2.10	0.85
1:F:370:SER:O	1:F:374:LEU:HB2	1.76	0.84
1:C:367:LYS:NZ	1:C:466:CYS:HA	1.94	0.83
1:D:14:LEU:HD13	1:D:212:ILE:HD12	1.59	0.83
1:F:91:VAL:HG11	1:F:101:ILE:HD13	1.60	0.83
1:E:160:ILE:HD11	1:E:193:GLN:O	1.81	0.81
1:D:192:TYR:CD1	1:D:234:TYR:HD2	1.97	0.81
1:A:272:ASN:H	1:A:272:ASN:ND2	1.75	0.81
1:B:274:VAL:HG23	1:B:275:HIS:HD2	1.46	0.81
1:F:276:GLN:HG3	1:F:292:MET:CE	2.11	0.81
1:E:58:ALA:HB1	1:E:84:ILE:HD13	1.63	0.81
1:A:282:VAL:HG21	1:A:467:SER:HB3	1.63	0.80
1:F:35:LEU:HD22	1:F:70:VAL:HG11	1.63	0.80
1:D:512:SER:HA	1:D:515:VAL:HG12	1.63	0.80
1:F:15:VAL:HB	1:F:209:VAL:HG22	1.63	0.80
1:B:495:LEU:HD22	1:B:521:LEU:HD23	1.64	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:342:VAL:HG23	1:D:343:GLY:H	1.44	0.80
1:D:154:MET:HG2	1:D:158:GLY:HA3	1.62	0.79
1:F:74:ILE:HD11	1:F:84:ILE:HD11	1.64	0.79
1:D:77:ARG:CG	1:D:77:ARG:HH11	1.96	0.79
1:E:78:ILE:HD13	1:E:96:MET:HE1	1.64	0.79
1:F:271:THR:HA	1:F:313:ASN:HB3	1.64	0.79
1:B:274:VAL:HG23	1:B:275:HIS:CD2	2.17	0.79
1:E:328:ARG:HH11	1:E:328:ARG:CG	1.95	0.79
1:B:339:PHE:CE2	1:B:341:PRO:HG3	2.19	0.78
1:B:154:MET:HG2	1:B:158:GLY:HA3	1.66	0.78
1:C:282:VAL:HG21	1:C:467:SER:HB3	1.65	0.78
1:A:20:MET:HG2	1:A:214:ALA:HB2	1.66	0.78
1:B:343:GLY:CA	1:B:350:ARG:HD3	2.13	0.78
1:C:78:ILE:HG21	1:C:96:MET:HE1	1.64	0.78
1:C:79:ASP:HB3	1:D:79:ASP:HB3	1.65	0.77
1:A:367:LYS:HZ1	1:A:466:CYS:HA	1.48	0.77
1:C:44:ILE:HG13	1:C:72:LEU:HD11	1.64	0.77
1:E:467:SER:HB2	1:E:496:TYR:CE1	2.17	0.77
1:F:154:MET:HG2	1:F:158:GLY:HA3	1.66	0.77
1:F:252:GLU:O	1:F:256:ILE:HD13	1.84	0.77
1:A:192:TYR:HD1	1:A:234:TYR:HD2	1.33	0.77
1:A:253:ILE:HD11	1:A:494:MET:HE2	1.67	0.77
1:A:337:ILE:N	1:A:337:ILE:HD12	2.00	0.77
1:C:328:ARG:HG3	1:C:328:ARG:HH11	1.49	0.76
1:D:281:ASN:HB3	1:D:518:ILE:HD13	1.67	0.76
1:F:276:GLN:HG3	1:F:292:MET:HE2	1.65	0.76
1:E:186:ASN:HD22	1:E:186:ASN:C	1.89	0.76
1:F:274:VAL:HG23	1:F:275:HIS:HD2	1.50	0.76
1:B:314:THR:HG21	1:B:354:ASN:HD21	1.48	0.75
1:B:475:MET:CE	1:B:495:LEU:HD12	2.17	0.75
1:B:78:ILE:HG21	1:B:96:MET:CE	2.14	0.75
1:C:187:ILE:HG23	1:C:206:ILE:CD1	2.16	0.75
1:B:191:LEU:HD22	1:B:206:ILE:HD11	1.68	0.75
1:B:253:ILE:O	1:B:257:ILE:HG13	1.87	0.75
1:D:437:THR:O	1:D:439:GLY:N	2.20	0.75
1:B:495:LEU:CD2	1:B:521:LEU:HD23	2.16	0.74
1:E:77:ARG:HG2	1:E:77:ARG:NH1	1.84	0.74
1:F:268:GLN:HB3	1:F:310:LEU:HD12	1.67	0.74
1:D:272:ASN:H	1:D:272:ASN:ND2	1.86	0.74
1:E:44:ILE:HG13	1:E:72:LEU:HD11	1.68	0.74
1:C:154:MET:HG2	1:C:158:GLY:HA3	1.68	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358:LEU:HD13	1:A:409:TYR:CE2	2.23	0.73
1:A:89:ILE:HD11	1:A:101:ILE:CG2	2.17	0.73
1:B:475:MET:HE1	1:B:495:LEU:HD12	1.70	0.73
1:A:78:ILE:HG21	1:A:96:MET:CE	2.17	0.73
1:F:424:ASP:HB2	1:F:486:PHE:CD1	2.23	0.73
1:F:124:LEU:HA	1:F:127:MET:HE2	1.70	0.73
1:F:527:GLU:HG3	1:F:527:GLU:O	1.87	0.73
1:E:98:ILE:N	1:E:99:PRO:HD2	2.04	0.73
1:A:115:VAL:HG13	1:A:120:GLU:HB2	1.70	0.73
1:A:479:GLN:NE2	1:A:483:GLY:HA3	2.03	0.73
1:F:73:ILE:HA	1:F:88:GLY:O	1.89	0.73
1:F:98:ILE:HD11	1:F:113:TRP:CD1	2.25	0.72
1:C:367:LYS:HZ1	1:C:466:CYS:HA	1.54	0.72
1:E:41:LEU:HD11	1:E:73:ILE:HD11	1.69	0.72
1:D:282:VAL:HG21	1:D:467:SER:HB3	1.69	0.72
1:F:299:VAL:HG21	1:F:326:ALA:HA	1.70	0.72
1:C:40:THR:HG21	1:C:226:ARG:HH21	1.53	0.72
1:E:274:VAL:HG23	1:E:275:HIS:HD2	1.52	0.72
1:F:437:THR:O	1:F:439:GLY:N	2.22	0.72
1:B:111:ILE:CG2	1:B:132:VAL:HA	2.19	0.72
1:B:115:VAL:HA	1:B:120:GLU:OE1	1.90	0.72
1:C:256:ILE:HG22	1:C:475:MET:HE1	1.71	0.72
1:F:59:LEU:HD21	1:F:84:ILE:HB	1.70	0.72
1:C:437:THR:O	1:C:439:GLY:N	2.22	0.72
1:E:77:ARG:HH11	1:E:77:ARG:CG	2.00	0.72
1:F:257:ILE:HD11	1:F:533:TRP:HH2	1.53	0.71
1:E:184:PRO:HD3	1:E:211:ASP:OD1	1.90	0.71
1:A:8:PHE:CE2	1:A:110:VAL:CG1	2.72	0.71
1:E:8:PHE:CE2	1:E:110:VAL:HG11	2.25	0.71
1:E:274:VAL:HG23	1:E:275:HIS:CD2	2.26	0.71
1:C:484:ASN:ND2	1:C:487:HIS:H	1.89	0.71
1:B:266:LEU:HD23	1:B:305:ILE:HG21	1.71	0.71
1:C:96:MET:CE	1:C:101:ILE:HG12	2.19	0.70
1:D:270:ILE:HD12	1:D:310:LEU:HD11	1.71	0.70
1:F:373:ILE:HG13	1:F:415:CYS:HB2	1.73	0.70
1:E:276:GLN:HG3	1:E:292:MET:HE3	1.73	0.70
1:A:342:VAL:HG23	1:A:342:VAL:O	1.91	0.70
1:E:271:THR:HA	1:E:313:ASN:HB3	1.73	0.70
1:D:16:THR:O	1:D:45:ARG:HB3	1.91	0.70
1:C:21:ILE:HD11	1:C:27:LEU:HD12	1.74	0.70
1:A:89:ILE:HD11	1:A:101:ILE:HG21	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:28:TYR:HE1	1:B:64:LEU:HB2	1.55	0.70
1:E:314:THR:HG21	1:E:354:ASN:ND2	2.06	0.70
1:B:484:ASN:HD21	1:B:487:HIS:H	1.40	0.70
1:A:370:SER:O	1:A:374:LEU:HB2	1.91	0.70
1:B:314:THR:HG21	1:B:354:ASN:ND2	2.07	0.69
1:C:271:THR:HA	1:C:313:ASN:HB3	1.72	0.69
1:F:520:ALA:O	1:F:524:LEU:HB2	1.92	0.69
1:C:241:LEU:O	1:C:428:GLU:HA	1.92	0.69
1:F:420:ASP:OD2	1:F:497:LYS:HD3	1.92	0.69
1:A:420:ASP:OD2	1:A:497:LYS:HD3	1.92	0.69
1:D:98:ILE:HG21	1:D:132:VAL:HG22	1.73	0.69
1:D:97:PRO:O	1:D:101:ILE:HG13	1.93	0.69
1:F:124:LEU:HA	1:F:127:MET:CE	2.22	0.69
1:A:44:ILE:HG13	1:A:72:LEU:HD11	1.73	0.69
1:A:91:VAL:HG11	1:A:101:ILE:HD13	1.73	0.69
1:C:40:THR:HG21	1:C:226:ARG:NH2	2.08	0.69
1:C:377:ALA:HB2	1:C:405:VAL:HG23	1.75	0.69
1:F:156:THR:HG21	1:F:193:GLN:HG3	1.75	0.69
1:B:78:ILE:HB	1:B:89:ILE:HD13	1.73	0.68
1:C:358:LEU:HD23	1:C:363:PHE:HE1	1.58	0.68
1:F:247:LEU:HG	1:F:539:HIS:NE2	2.08	0.68
1:D:367:LYS:NZ	1:D:466:CYS:HA	2.08	0.68
1:D:373:ILE:HG13	1:D:415:CYS:HB2	1.73	0.68
1:A:343:GLY:CA	1:A:350:ARG:HD3	2.23	0.68
1:C:101:ILE:O	1:C:105:VAL:HG22	1.93	0.68
1:B:407:PHE:CE2	1:B:410:LYS:HE3	2.27	0.68
1:A:35:LEU:HD12	1:A:64:LEU:HD13	1.74	0.68
1:D:183:HIS:H	1:D:186:ASN:ND2	1.89	0.68
1:E:74:ILE:HD11	1:E:84:ILE:HD11	1.76	0.68
1:D:367:LYS:HZ3	1:D:466:CYS:HA	1.59	0.68
1:A:328:ARG:HH11	1:A:328:ARG:CG	2.06	0.68
1:D:313:ASN:C	1:D:313:ASN:HD22	1.96	0.68
1:A:274:VAL:HG23	1:A:275:HIS:HD2	1.57	0.68
1:B:192:TYR:HD1	1:B:234:TYR:HD2	1.42	0.68
1:F:337:ILE:HG21	1:F:363:PHE:CD2	2.29	0.68
1:F:486:PHE:O	1:F:490:VAL:HG23	1.93	0.67
1:A:347:THR:HG21	1:C:298:GLU:HG3	1.75	0.67
1:B:77:ARG:HH11	1:F:77:ARG:NH1	1.91	0.67
1:F:337:ILE:HG21	1:F:363:PHE:HD2	1.58	0.67
1:D:44:ILE:HG13	1:D:72:LEU:HD11	1.76	0.67
1:A:400:GLN:O	1:A:404:ILE:HG13	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:154:MET:HG3	1:E:158:GLY:HA3	1.75	0.67
1:A:8:PHE:HE2	1:A:110:VAL:CG1	2.07	0.67
1:E:256:ILE:HD13	1:E:488:ALA:HA	1.76	0.67
1:F:8:PHE:CE2	1:F:110:VAL:CG2	2.76	0.67
1:D:484:ASN:HD22	1:D:487:HIS:H	1.41	0.67
1:C:294:GLU:OE1	1:C:318:ALA:HB2	1.95	0.67
1:E:520:ALA:O	1:E:524:LEU:HB2	1.94	0.67
1:C:527:GLU:O	1:C:527:GLU:HG3	1.95	0.67
1:F:98:ILE:HD13	1:F:101:ILE:HD12	1.77	0.67
1:D:192:TYR:HD1	1:D:234:TYR:CD2	2.08	0.67
1:E:467:SER:HB2	1:E:496:TYR:HE1	1.58	0.67
1:E:110:VAL:HG23	1:E:133:ASP:CB	2.25	0.67
1:F:15:VAL:HB	1:F:209:VAL:CG2	2.24	0.67
1:D:298:GLU:HG2	1:F:347:THR:HG21	1.75	0.67
1:D:308:ALA:O	1:D:335:ARG:HD3	1.95	0.67
1:B:144:LEU:H	1:B:144:LEU:HD12	1.59	0.67
1:F:125:SER:C	1:F:127:MET:H	1.98	0.66
1:A:96:MET:CE	1:A:101:ILE:HG12	2.26	0.66
1:B:322:MET:HG3	1:B:323:LEU:N	2.10	0.66
1:A:512:SER:HA	1:A:515:VAL:HG12	1.77	0.66
1:E:472:ILE:O	1:E:476:ILE:HG13	1.95	0.66
1:D:394:SER:OG	1:D:395:ASN:N	2.28	0.66
1:B:433:LEU:O	1:B:434:SER:HB2	1.95	0.66
1:F:427:ILE:O	1:F:427:ILE:HG22	1.94	0.66
1:F:358:LEU:HD13	1:F:409:TYR:CE2	2.31	0.66
1:B:250:THR:HG23	1:B:530:PRO:HB2	1.77	0.66
1:F:115:VAL:HG13	1:F:120:GLU:HB2	1.77	0.66
1:E:328:ARG:HG2	1:E:328:ARG:HH11	1.61	0.66
1:F:8:PHE:HE2	1:F:110:VAL:CG2	2.07	0.65
1:B:14:LEU:HD11	1:B:213:ILE:HD11	1.77	0.65
1:E:342:VAL:HG23	1:E:343:GLY:H	1.61	0.65
1:F:74:ILE:CD1	1:F:84:ILE:HD11	2.27	0.65
1:B:28:TYR:CE1	1:B:64:LEU:HG	2.30	0.65
1:E:276:GLN:HG3	1:E:292:MET:CE	2.25	0.65
1:B:420:ASP:OD2	1:B:497:LYS:HD3	1.97	0.65
1:E:125:SER:C	1:E:127:MET:H	1.99	0.65
1:E:256:ILE:HG22	1:E:475:MET:HE1	1.79	0.65
1:B:520:ALA:O	1:B:524:LEU:HB2	1.96	0.65
1:A:145:THR:HB	2:A:541:3NM:H7	1.77	0.65
1:B:467:SER:HB2	1:B:496:TYR:CE1	2.31	0.65
1:C:495:LEU:HD11	1:C:525:THR:CG2	2.25	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:ILE:HD12	1:A:81:ALA:HA	1.78	0.65
1:A:15:VAL:HG22	1:A:43:GLN:HB3	1.78	0.65
1:B:197:SER:O	1:B:442:VAL:HG23	1.96	0.65
1:F:442:VAL:O	1:F:445:ILE:HG12	1.97	0.65
1:A:318:ALA:HB1	1:A:322:MET:HG2	1.79	0.65
1:A:322:MET:HG3	1:A:323:LEU:HD23	1.78	0.65
1:B:485:LEU:O	1:B:489:VAL:HG23	1.95	0.65
1:E:366:ILE:CD1	1:E:411:THR:HG21	2.26	0.65
1:B:276:GLN:HG3	1:B:292:MET:CE	2.26	0.65
1:A:292:MET:HE2	1:B:274:VAL:HG11	1.76	0.65
1:E:269:HIS:HB3	1:E:271:THR:HG22	1.79	0.65
1:F:89:ILE:HD11	1:F:101:ILE:CG2	2.27	0.64
1:C:358:LEU:HD23	1:C:363:PHE:CE1	2.31	0.64
1:A:433:LEU:HD12	1:A:433:LEU:N	2.11	0.64
1:A:187:ILE:HG12	1:A:206:ILE:CD1	2.23	0.64
1:B:77:ARG:HH11	1:B:77:ARG:HG2	1.62	0.64
1:C:298:GLU:HG2	1:C:302:LEU:HD11	1.78	0.64
1:C:264:ARG:N	1:C:265:PRO:HD3	2.12	0.64
1:D:78:ILE:HG21	1:D:96:MET:CE	2.27	0.64
1:B:20:MET:HE3	1:B:213:ILE:HB	1.78	0.64
1:A:253:ILE:HD11	1:A:494:MET:CE	2.27	0.64
1:E:256:ILE:HG12	1:E:479:GLN:OE1	1.98	0.64
1:A:74:ILE:HD11	1:A:84:ILE:HD11	1.79	0.64
1:A:78:ILE:O	1:A:81:ALA:HB3	1.97	0.64
1:B:366:ILE:CD1	1:B:411:THR:HG21	2.25	0.64
1:D:283:THR:HB	1:D:290:PRO:HG3	1.80	0.64
1:B:328:ARG:CG	1:B:328:ARG:HH11	2.10	0.64
1:B:88:GLY:HA3	1:B:110:VAL:CG1	2.28	0.64
1:A:299:VAL:HG21	1:A:326:ALA:CA	2.25	0.64
1:C:484:ASN:HD22	1:C:487:HIS:H	1.44	0.64
1:B:192:TYR:CD1	1:B:234:TYR:HD2	2.16	0.64
1:B:17:ASP:HB3	1:B:20:MET:HE1	1.79	0.64
1:C:427:ILE:O	1:C:427:ILE:HG22	1.98	0.64
1:C:339:PHE:CE2	1:C:341:PRO:HG3	2.33	0.64
1:B:183:HIS:O	1:B:187:ILE:HD12	1.97	0.64
1:B:267:VAL:HG12	1:B:269:HIS:CE1	2.32	0.63
1:E:299:VAL:CG2	1:E:326:ALA:HA	2.28	0.63
1:E:187:ILE:HG23	1:E:206:ILE:CD1	2.28	0.63
1:F:269:HIS:HB2	1:F:292:MET:SD	2.38	0.63
1:C:249:THR:OG1	1:C:252:GLU:HG3	1.98	0.63
1:A:274:VAL:HG23	1:A:275:HIS:CD2	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:367:LYS:HZ2	1:D:469:GLY:H	1.45	0.63
1:E:20:MET:HG2	1:E:20:MET:O	1.98	0.63
1:E:79:ASP:OD1	1:E:80:VAL:N	2.32	0.63
1:C:187:ILE:HG23	1:C:206:ILE:HD13	1.79	0.63
1:C:256:ILE:HG22	1:C:475:MET:CE	2.27	0.63
1:B:145:THR:HB	2:B:541:3NM:H7	1.81	0.63
1:A:172:HIS:O	1:A:175:ARG:NH2	2.32	0.63
1:A:256:ILE:O	1:A:260:THR:HG22	1.97	0.63
1:D:420:ASP:OD2	1:D:497:LYS:HD3	1.98	0.63
1:B:72:LEU:HD12	1:B:73:ILE:N	2.14	0.63
1:D:299:VAL:CG2	1:D:326:ALA:HA	2.22	0.63
1:B:35:LEU:CD2	1:B:70:VAL:HG11	2.29	0.63
1:A:479:GLN:HE21	1:A:483:GLY:HA3	1.61	0.63
1:E:168:ARG:HG2	1:E:168:ARG:O	1.98	0.63
1:C:275:HIS:CD2	1:C:275:HIS:H	2.17	0.62
1:C:38:GLY:O	1:C:40:THR:HG23	1.98	0.62
1:A:88:GLY:HA3	1:A:110:VAL:HG13	1.79	0.62
1:A:366:ILE:HD12	1:A:411:THR:HG21	1.80	0.62
1:F:97:PRO:O	1:F:101:ILE:HG13	1.99	0.62
1:A:77:ARG:NH1	1:E:77:ARG:NH1	2.48	0.62
1:B:189:ARG:O	1:B:193:GLN:HG2	1.99	0.62
1:A:187:ILE:HD13	1:A:225:LEU:CD2	2.29	0.62
1:A:476:ILE:HD13	1:A:485:LEU:HD11	1.80	0.62
1:B:275:HIS:N	1:B:275:HIS:CD2	2.67	0.62
1:F:187:ILE:HG23	1:F:206:ILE:HD12	1.80	0.62
1:E:495:LEU:HD22	1:E:521:LEU:HD23	1.80	0.62
1:F:484:ASN:HD22	1:F:487:HIS:H	1.47	0.62
1:A:269:HIS:HB2	1:A:292:MET:SD	2.40	0.62
1:B:533:TRP:HB3	1:B:535:PRO:HD2	1.80	0.62
1:B:513:PHE:CD2	1:B:513:PHE:C	2.73	0.62
1:A:96:MET:HE2	1:A:101:ILE:HG12	1.82	0.61
1:B:310:LEU:HD23	1:B:337:ILE:HG23	1.82	0.61
1:B:195:VAL:HG12	1:B:202:SER:HB2	1.80	0.61
1:D:399:ILE:HD13	1:D:421:PHE:CD2	2.35	0.61
1:B:498:ALA:O	1:B:502:ILE:HG13	2.00	0.61
1:C:78:ILE:HG21	1:C:96:MET:HE2	1.78	0.61
1:D:8:PHE:HE2	1:D:110:VAL:HB	1.65	0.61
1:D:276:GLN:HG3	1:D:292:MET:CE	2.29	0.61
1:D:51:THR:O	1:D:55:ILE:HG13	2.00	0.61
1:B:364:SER:HB3	1:B:485:LEU:HD21	1.83	0.61
1:E:484:ASN:HD22	1:E:487:HIS:H	1.47	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:HIS:O	1:A:187:ILE:HD12	2.01	0.61
1:F:308:ALA:O	1:F:335:ARG:HD3	2.01	0.61
1:A:272:ASN:HD21	1:A:313:ASN:HD22	1.49	0.61
1:A:468:LEU:O	1:A:472:ILE:HG13	2.01	0.61
1:D:399:ILE:HD11	1:D:421:PHE:CE2	2.36	0.61
1:E:89:ILE:HG13	1:E:89:ILE:O	1.99	0.61
1:A:272:ASN:N	1:A:272:ASN:ND2	2.44	0.60
1:A:59:LEU:HD21	1:A:84:ILE:HB	1.83	0.60
1:B:193:GLN:NE2	1:B:362:GLN:HE21	1.99	0.60
1:A:324:LYS:HB2	1:A:360:PHE:CE1	2.36	0.60
1:B:286:LEU:HD11	1:B:471:THR:HG23	1.83	0.60
1:B:299:VAL:HG21	1:B:326:ALA:HA	1.84	0.60
1:C:365:CYS:HA	1:C:412:VAL:O	2.01	0.60
1:A:144:LEU:HD12	1:A:144:LEU:H	1.65	0.60
1:E:136:GLY:HA2	1:E:177:VAL:HG23	1.84	0.60
1:B:79:ASP:OD1	1:B:80:VAL:N	2.35	0.60
1:F:35:LEU:HD12	1:F:64:LEU:HD13	1.83	0.60
1:F:59:LEU:CD2	1:F:84:ILE:HB	2.32	0.60
1:D:424:ASP:HB2	1:D:486:PHE:CD1	2.36	0.60
1:A:424:ASP:HB3	1:A:446:PRO:HG2	1.83	0.60
1:D:79:ASP:OD1	1:D:80:VAL:N	2.35	0.60
1:A:509:GLY:HA2	1:C:522:TYR:CD2	2.36	0.60
1:E:437:THR:O	1:E:439:GLY:N	2.35	0.60
1:A:313:ASN:HD21	1:A:342:VAL:CG2	2.07	0.60
1:D:298:GLU:OE1	1:F:347:THR:HG21	2.00	0.60
1:F:296:GLN:HG2	1:F:322:MET:HB2	1.83	0.60
1:C:40:THR:CG2	1:C:226:ARG:HH21	2.15	0.60
1:A:305:ILE:HG23	1:A:306:PRO:HD2	1.83	0.60
1:A:77:ARG:HG2	1:A:77:ARG:HH11	1.67	0.59
1:A:337:ILE:H	1:A:337:ILE:HD12	1.67	0.59
1:D:74:ILE:HD11	1:D:84:ILE:HD11	1.84	0.59
1:D:328:ARG:HG3	1:D:328:ARG:HH11	1.67	0.59
1:E:135:ILE:CG1	1:E:176:THR:HG22	2.32	0.59
1:D:408:LYS:HD3	1:D:409:TYR:CZ	2.37	0.59
1:D:180:GLY:HA2	2:D:541:3NM:H7A	1.84	0.59
1:F:91:VAL:HG11	1:F:101:ILE:CD1	2.31	0.59
1:A:192:TYR:HD1	1:A:234:TYR:CD2	2.18	0.59
1:D:137:VAL:O	1:D:138:GLY:O	2.20	0.59
1:A:77:ARG:NH1	1:E:77:ARG:HH11	2.01	0.59
1:D:342:VAL:HG23	1:D:343:GLY:N	2.17	0.59
1:A:42:VAL:O	1:A:72:LEU:HD12	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:265:PRO:HD2	1:E:288:SER:OG	2.02	0.59
1:F:451:GLU:HG2	1:F:452:ALA:N	2.17	0.59
1:C:250:THR:HG23	1:C:530:PRO:HB2	1.85	0.59
1:B:20:MET:HG2	1:B:20:MET:O	2.02	0.59
1:D:278:PHE:O	1:D:281:ASN:HB2	2.02	0.59
1:A:416:THR:HG21	1:A:468:LEU:HD23	1.85	0.59
1:C:370:SER:O	1:C:374:LEU:HB2	2.02	0.59
1:C:89:ILE:HD11	1:C:101:ILE:HD13	1.84	0.59
1:D:187:ILE:HG23	1:D:206:ILE:CD1	2.32	0.58
1:A:358:LEU:HD23	1:A:363:PHE:HE1	1.68	0.58
1:C:276:GLN:NE2	1:C:292:MET:HB3	2.18	0.58
1:B:125:SER:C	1:B:127:MET:H	2.07	0.58
1:F:394:SER:OG	1:F:395:ASN:N	2.35	0.58
1:A:79:ASP:OD1	1:A:80:VAL:N	2.36	0.58
1:A:73:ILE:HG23	1:A:88:GLY:C	2.24	0.58
1:E:295:ILE:HG22	1:E:298:GLU:HB2	1.85	0.58
1:D:274:VAL:HG23	1:D:275:HIS:CD2	2.38	0.58
1:C:15:VAL:HB	1:C:209:VAL:HG22	1.84	0.58
1:C:8:PHE:CE2	1:C:110:VAL:HG21	2.38	0.58
1:F:109:MET:HG2	1:F:110:VAL:N	2.19	0.58
1:C:342:VAL:HG23	1:C:343:GLY:H	1.69	0.58
1:F:424:ASP:HB3	1:F:446:PRO:HG2	1.85	0.58
1:F:479:GLN:HE21	1:F:484:ASN:H	1.50	0.58
1:A:283:THR:HB	1:A:290:PRO:HG3	1.86	0.58
1:B:343:GLY:HA3	1:B:350:ARG:CD	2.20	0.58
1:E:74:ILE:HD12	1:E:81:ALA:HA	1.84	0.58
1:E:468:LEU:O	1:E:472:ILE:HG13	2.04	0.58
1:B:87:ASP:O	1:B:110:VAL:HG12	2.04	0.58
1:E:347:THR:HG21	1:F:298:GLU:HG2	1.85	0.58
1:A:96:MET:O	1:A:101:ILE:HD11	2.03	0.58
1:E:187:ILE:HG12	1:E:206:ILE:HD13	1.85	0.58
1:F:533:TRP:C	1:F:535:PRO:HD2	2.23	0.58
1:C:35:LEU:HD22	1:C:70:VAL:HG11	1.85	0.58
1:E:266:LEU:HD11	1:E:291:ILE:HG13	1.86	0.58
1:A:298:GLU:CG	1:B:347:THR:HG21	2.33	0.58
1:A:367:LYS:HZ2	1:A:466:CYS:HA	1.68	0.58
1:E:328:ARG:HG2	1:E:328:ARG:NH1	2.19	0.58
1:D:248:THR:HG23	1:D:487:HIS:ND1	2.18	0.58
1:E:250:THR:HG23	1:E:530:PRO:HB2	1.86	0.58
1:C:328:ARG:CG	1:C:328:ARG:HH11	2.13	0.57
1:E:116:GLY:C	1:E:117:PHE:HD2	2.07	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:77:ARG:NH1	1:F:77:ARG:NH1	2.52	0.57
1:B:234:TYR:HE2	1:B:362:GLN:HG3	1.69	0.57
1:B:115:VAL:HG13	1:B:120:GLU:CB	2.31	0.57
1:B:422:ILE:HG22	1:B:486:PHE:HE1	1.69	0.57
1:A:534:ALA:N	1:A:535:PRO:CD	2.67	0.57
1:B:367:LYS:NZ	1:B:466:CYS:HA	2.19	0.57
1:A:117:PHE:N	1:A:117:PHE:CD2	2.72	0.57
1:E:15:VAL:HB	1:E:209:VAL:HG22	1.84	0.57
1:B:89:ILE:O	1:B:89:ILE:HG13	2.05	0.57
1:D:451:GLU:HG2	1:D:452:ALA:N	2.19	0.57
1:A:272:ASN:HD21	1:A:313:ASN:ND2	2.01	0.57
1:F:276:GLN:HG3	1:F:292:MET:HE3	1.85	0.57
1:B:271:THR:HA	1:B:313:ASN:HB3	1.85	0.57
1:B:109:MET:HG2	1:B:110:VAL:H	1.70	0.57
1:B:256:ILE:O	1:B:260:THR:HG22	2.05	0.57
1:D:348:GLU:OE1	1:D:348:GLU:HA	2.05	0.57
1:B:322:MET:HE2	1:B:326:ALA:HB2	1.86	0.57
1:D:89:ILE:HD11	1:D:101:ILE:HG21	1.86	0.57
1:C:20:MET:HG2	1:C:214:ALA:HB2	1.87	0.57
1:C:21:ILE:HD11	1:C:27:LEU:CD1	2.34	0.57
1:D:98:ILE:HG21	1:D:132:VAL:CG2	2.35	0.57
1:B:276:GLN:HG3	1:B:292:MET:HE3	1.84	0.57
1:A:250:THR:HG23	1:A:530:PRO:HB2	1.86	0.57
1:C:308:ALA:O	1:C:335:ARG:NH1	2.37	0.57
1:A:495:LEU:HD22	1:A:521:LEU:CD2	2.34	0.57
1:A:119:GLU:OE1	1:A:119:GLU:N	2.28	0.57
1:E:20:MET:CG	1:E:20:MET:O	2.53	0.57
1:F:187:ILE:HG23	1:F:206:ILE:CD1	2.34	0.57
1:C:125:SER:CB	1:C:169:ASN:HD22	2.18	0.57
1:A:192:TYR:CD1	1:A:234:TYR:HD2	2.17	0.56
1:F:274:VAL:HG23	1:F:275:HIS:CD2	2.37	0.56
1:D:151:LYS:O	1:D:152:ALA:HB3	2.04	0.56
1:F:468:LEU:O	1:F:472:ILE:HG13	2.05	0.56
1:F:475:MET:CE	1:F:495:LEU:HD12	2.35	0.56
1:F:89:ILE:HD11	1:F:101:ILE:HG21	1.87	0.56
1:A:89:ILE:O	1:A:89:ILE:HG13	2.04	0.56
1:E:59:LEU:HD21	1:E:84:ILE:HB	1.87	0.56
1:B:475:MET:HE2	1:B:495:LEU:HD12	1.88	0.56
1:D:101:ILE:O	1:D:105:VAL:HG22	2.05	0.56
1:A:247:LEU:HD22	1:A:537:LEU:HG	1.86	0.56
1:D:65:CYS:HB3	1:D:70:VAL:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:407:PHE:HE2	1:A:427:ILE:HD11	1.70	0.56
1:D:64:LEU:HD22	1:D:64:LEU:O	2.04	0.56
1:E:283:THR:HG23	1:E:474:CYS:SG	2.45	0.56
1:C:17:ASP:HB3	1:C:20:MET:CE	2.35	0.56
1:B:190:VAL:O	1:B:194:CYS:HB2	2.05	0.56
1:C:367:LYS:HZ2	1:C:466:CYS:HA	1.67	0.56
1:C:269:HIS:HB2	1:C:292:MET:SD	2.45	0.56
1:C:520:ALA:O	1:C:524:LEU:HB2	2.04	0.56
1:D:333:VAL:O	1:D:333:VAL:HG12	2.04	0.56
1:A:280:ALA:HB2	1:A:292:MET:CE	2.36	0.56
1:D:115:VAL:O	1:D:138:GLY:N	2.32	0.56
1:B:10:TYR:CE1	1:B:175:ARG:HG3	2.41	0.56
1:A:225:LEU:O	1:A:229:ILE:HG13	2.04	0.56
1:C:211:ASP:OD1	1:C:225:LEU:HD21	2.05	0.56
1:A:77:ARG:HH12	1:E:77:ARG:HH11	1.52	0.56
1:A:32:GLU:HG3	1:A:64:LEU:HD11	1.87	0.56
1:D:14:LEU:CD1	1:D:212:ILE:HD12	2.33	0.56
1:D:75:ASN:O	1:D:77:ARG:N	2.34	0.56
1:D:272:ASN:N	1:D:272:ASN:ND2	2.54	0.56
1:D:347:THR:OG1	1:D:350:ARG:HB2	2.06	0.56
1:B:534:ALA:N	1:B:535:PRO:HD2	2.20	0.56
1:F:15:VAL:HG22	1:F:43:GLN:NE2	2.19	0.56
1:F:55:ILE:HG23	1:F:84:ILE:CG2	2.36	0.56
1:B:318:ALA:HB1	1:B:322:MET:HG2	1.86	0.56
1:C:44:ILE:HD11	1:C:61:ILE:CG2	2.35	0.56
1:B:468:LEU:O	1:B:472:ILE:HG13	2.06	0.56
1:E:275:HIS:HB3	1:E:466:CYS:SG	2.46	0.55
1:F:59:LEU:HD21	1:F:84:ILE:CB	2.36	0.55
1:C:249:THR:HG23	1:C:252:GLU:OE1	2.06	0.55
1:E:116:GLY:O	1:E:117:PHE:HD2	1.89	0.55
1:B:76:ASP:HA	1:B:91:VAL:HG12	1.88	0.55
1:D:343:GLY:HA3	1:D:350:ARG:HD3	1.88	0.55
1:A:192:TYR:CE2	1:A:410:LYS:HG3	2.42	0.55
1:D:486:PHE:O	1:D:490:VAL:HG23	2.06	0.55
1:D:8:PHE:CD1	1:D:71:PRO:HG2	2.42	0.55
1:C:115:VAL:HG13	1:C:120:GLU:HB2	1.88	0.55
1:C:51:THR:O	1:C:55:ILE:HG13	2.04	0.55
1:E:294:GLU:HA	1:E:322:MET:HE1	1.88	0.55
1:F:400:GLN:O	1:F:404:ILE:HG13	2.06	0.55
1:A:8:PHE:CZ	1:A:110:VAL:HG11	2.40	0.55
1:A:117:PHE:N	1:A:117:PHE:HD2	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:VAL:O	1:A:35:LEU:HG	2.06	0.55
1:B:257:ILE:HB	1:B:528:ASN:ND2	2.21	0.55
1:E:269:HIS:HB3	1:E:271:THR:CG2	2.36	0.55
1:F:495:LEU:HD22	1:F:521:LEU:CD2	2.37	0.55
1:D:247:LEU:HD21	1:D:538:THR:O	2.05	0.55
1:A:274:VAL:CG1	1:C:292:MET:HG3	2.37	0.55
1:C:74:ILE:HD12	1:C:86:ALA:HB2	1.89	0.55
1:A:98:ILE:HD11	1:A:113:TRP:NE1	2.22	0.55
1:F:16:THR:O	1:F:45:ARG:HB3	2.05	0.55
1:A:35:LEU:HD12	1:A:64:LEU:CD1	2.37	0.55
1:E:59:LEU:CD2	1:E:84:ILE:HB	2.36	0.55
1:B:323:LEU:HD13	1:B:357:LEU:HD21	1.88	0.55
1:B:328:ARG:HG3	1:B:328:ARG:HH11	1.72	0.55
1:A:179:ILE:HG12	1:A:180:GLY:N	2.22	0.55
1:D:313:ASN:HD21	1:D:342:VAL:HG21	1.71	0.55
1:A:257:ILE:HA	1:A:260:THR:CG2	2.37	0.55
1:A:407:PHE:CE2	1:A:427:ILE:HD11	2.41	0.55
1:E:78:ILE:O	1:E:81:ALA:HB3	2.06	0.55
1:A:337:ILE:CD1	1:A:337:ILE:N	2.70	0.55
1:A:121:VAL:CG1	1:A:166:LEU:HD23	2.36	0.55
1:E:164:ASP:OD2	1:E:197:SER:HB2	2.07	0.55
1:F:96:MET:HE3	1:F:101:ILE:HG12	1.89	0.55
1:D:299:VAL:HG13	1:D:300:ASN:N	2.22	0.55
1:C:302:LEU:N	1:C:302:LEU:CD1	2.69	0.55
1:E:266:LEU:HD11	1:E:291:ILE:CG1	2.36	0.55
1:E:310:LEU:HD23	1:E:337:ILE:HD13	1.89	0.55
1:F:55:ILE:HG12	1:F:80:VAL:HG13	1.88	0.54
1:C:191:LEU:HB3	1:C:431:TYR:CD2	2.42	0.54
1:F:257:ILE:HD11	1:F:533:TRP:CH2	2.40	0.54
1:E:116:GLY:C	1:E:117:PHE:CD2	2.80	0.54
1:D:77:ARG:CG	1:D:77:ARG:NH1	2.63	0.54
1:B:88:GLY:HA3	1:B:110:VAL:HG12	1.89	0.54
1:B:97:PRO:O	1:B:101:ILE:HG13	2.08	0.54
1:B:183:HIS:C	1:B:187:ILE:HD12	2.27	0.54
1:A:62:LYS:HB2	1:A:72:LEU:HD23	1.89	0.54
1:A:328:ARG:HH11	1:A:328:ARG:HG3	1.72	0.54
1:C:394:SER:OG	1:C:395:ASN:N	2.40	0.54
1:E:135:ILE:HG13	1:E:176:THR:HG22	1.90	0.54
1:B:10:TYR:HE1	1:B:175:ARG:HG3	1.73	0.54
1:E:294:GLU:HA	1:E:322:MET:CE	2.37	0.54
1:A:484:ASN:HD22	1:A:487:HIS:H	1.56	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:11:SER:HB2	1:D:226:ARG:HH12	1.71	0.54
1:E:186:ASN:HD22	1:E:187:ILE:N	2.05	0.54
1:B:10:TYR:O	1:B:11:SER:C	2.46	0.54
1:B:78:ILE:CG2	1:B:96:MET:HE1	2.24	0.54
1:B:28:TYR:OH	1:B:64:LEU:HD23	2.08	0.54
1:B:187:ILE:HG12	1:B:206:ILE:HD13	1.89	0.54
1:E:424:ASP:HB3	1:E:446:PRO:HG2	1.89	0.54
1:E:314:THR:OG1	1:E:354:ASN:OD1	2.24	0.54
1:C:437:THR:C	1:C:439:GLY:N	2.60	0.54
1:C:296:GLN:HG3	1:C:322:MET:HB2	1.90	0.54
1:F:189:ARG:O	1:F:193:GLN:HG2	2.08	0.54
1:F:282:VAL:HG21	1:F:467:SER:HB3	1.90	0.54
1:C:296:GLN:O	1:C:299:VAL:HG12	2.07	0.54
1:C:58:ALA:HB1	1:C:84:ILE:HD13	1.90	0.54
1:B:210:SER:O	1:B:214:ALA:HB3	2.07	0.54
1:A:378:GLU:OE2	1:A:408:LYS:HE2	2.08	0.54
1:E:78:ILE:O	1:E:82:MET:HG3	2.08	0.54
1:E:449:ALA:O	1:E:537:LEU:HD12	2.08	0.54
1:F:43:GLN:HA	1:F:73:ILE:O	2.07	0.53
1:D:318:ALA:HB1	1:D:322:MET:HG2	1.88	0.53
1:F:299:VAL:HG21	1:F:326:ALA:CA	2.38	0.53
1:D:424:ASP:HB3	1:D:446:PRO:HG2	1.88	0.53
1:C:55:ILE:HG23	1:C:84:ILE:CG2	2.38	0.53
1:C:235:LYS:HE2	1:C:237:VAL:O	2.08	0.53
1:E:362:GLN:HE21	1:E:362:GLN:HA	1.72	0.53
1:B:342:VAL:HG23	1:B:343:GLY:H	1.73	0.53
1:B:294:GLU:OE1	1:B:318:ALA:HB2	2.09	0.53
1:B:187:ILE:HG23	1:B:206:ILE:CD1	2.38	0.53
1:F:125:SER:C	1:F:127:MET:N	2.61	0.53
1:F:358:LEU:HD23	1:F:363:PHE:CE1	2.44	0.53
1:F:358:LEU:HD23	1:F:363:PHE:HE1	1.71	0.53
1:D:197:SER:O	1:D:442:VAL:HG23	2.08	0.53
1:D:74:ILE:HD13	1:D:80:VAL:HG12	1.90	0.53
1:B:433:LEU:O	1:B:434:SER:CB	2.56	0.53
1:A:422:ILE:HD12	1:A:490:VAL:HG22	1.90	0.53
1:E:224:ILE:O	1:E:228:LEU:HD13	2.09	0.53
1:E:323:LEU:HD13	1:E:357:LEU:HD11	1.89	0.53
1:E:163:LEU:HD22	1:E:201:ARG:HD3	1.89	0.53
1:E:295:ILE:CG2	1:E:298:GLU:HB2	2.39	0.53
1:E:427:ILE:O	1:E:427:ILE:HG22	2.09	0.53
1:D:77:ARG:HG2	1:D:77:ARG:NH1	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:187:ILE:HD13	1:F:225:LEU:HD22	1.89	0.53
1:F:324:LYS:HB2	1:F:360:PHE:CE1	2.43	0.53
1:F:337:ILE:CG2	1:F:363:PHE:HD2	2.22	0.53
1:B:109:MET:HG2	1:B:110:VAL:N	2.24	0.53
1:A:55:ILE:HG23	1:A:84:ILE:CG2	2.39	0.53
1:A:299:VAL:HG21	1:A:326:ALA:CB	2.39	0.53
1:C:482:GLU:H	1:C:482:GLU:CD	2.12	0.53
1:D:260:THR:HA	1:D:478:GLY:HA3	1.91	0.53
1:A:110:VAL:HA	1:A:133:ASP:OD2	2.08	0.53
1:F:209:VAL:HB	2:F:541:3NM:O5	2.09	0.53
1:A:98:ILE:N	1:A:99:PRO:HD2	2.23	0.53
1:E:232:THR:HG22	1:E:431:TYR:O	2.09	0.53
1:D:78:ILE:HD11	1:D:104:LEU:HD12	1.91	0.53
1:D:437:THR:C	1:D:439:GLY:N	2.61	0.53
1:C:437:THR:O	1:C:438:ASN:C	2.47	0.53
1:D:121:VAL:HG13	1:D:166:LEU:HD23	1.90	0.53
1:F:144:LEU:H	1:F:144:LEU:HD12	1.73	0.53
1:B:119:GLU:H	1:B:119:GLU:CD	2.12	0.53
1:E:8:PHE:CE2	1:E:110:VAL:CG1	2.91	0.52
1:E:394:SER:OG	1:E:395:ASN:N	2.42	0.52
1:D:257:ILE:HD11	1:D:533:TRP:HH2	1.73	0.52
1:B:533:TRP:C	1:B:535:PRO:HD2	2.29	0.52
1:F:472:ILE:HG23	1:F:489:VAL:HG22	1.91	0.52
1:F:20:MET:HE3	1:F:214:ALA:HB2	1.91	0.52
1:B:27:LEU:O	1:B:31:VAL:HG23	2.10	0.52
1:B:437:THR:O	1:B:438:ASN:C	2.46	0.52
1:A:333:VAL:HG12	1:A:333:VAL:O	2.10	0.52
1:B:46:GLU:OE2	1:B:46:GLU:HA	2.08	0.52
1:A:91:VAL:HG11	1:A:101:ILE:CD1	2.38	0.52
1:B:16:THR:HG23	1:B:27:LEU:HD11	1.91	0.52
1:D:115:VAL:HG13	1:D:120:GLU:CB	2.39	0.52
1:C:123:GLU:O	1:C:127:MET:HG3	2.09	0.52
1:F:433:LEU:O	1:F:434:SER:OG	2.21	0.52
1:F:176:THR:O	1:F:204:ASP:HB2	2.09	0.52
1:F:42:VAL:HG12	1:F:72:LEU:CD1	2.39	0.52
1:B:283:THR:HB	1:B:290:PRO:HG3	1.90	0.52
1:A:121:VAL:HG13	1:A:166:LEU:HD23	1.92	0.52
1:C:141:PHE:HB3	1:C:142:PRO:CD	2.40	0.52
1:C:104:LEU:O	1:C:105:VAL:HG13	2.10	0.52
1:F:424:ASP:O	1:F:445:ILE:HB	2.09	0.52
1:C:260:THR:HA	1:C:478:GLY:HA3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:442:VAL:O	1:A:445:ILE:HG12	2.10	0.52
1:F:495:LEU:HD22	1:F:521:LEU:HD23	1.91	0.52
1:B:427:ILE:HG22	1:B:427:ILE:O	2.09	0.52
1:E:144:LEU:HD12	1:E:144:LEU:H	1.74	0.52
1:E:256:ILE:HG22	1:E:475:MET:CE	2.40	0.52
1:A:10:TYR:O	1:A:11:SER:C	2.48	0.52
1:C:220:LYS:O	1:C:224:ILE:HG13	2.10	0.52
1:E:115:VAL:HG13	1:E:120:GLU:HB2	1.92	0.52
1:F:119:GLU:O	1:F:123:GLU:HG3	2.09	0.52
1:D:21:ILE:HD11	1:D:27:LEU:HD13	1.92	0.52
1:F:80:VAL:O	1:F:84:ILE:HG12	2.10	0.52
1:B:138:GLY:HA3	1:B:154:MET:CE	2.39	0.52
1:C:112:GLY:HA3	1:C:134:TYR:CZ	2.45	0.52
1:C:419:PHE:CE1	1:C:451:GLU:HB2	2.45	0.52
1:F:78:ILE:HD12	1:F:96:MET:HE1	1.91	0.51
1:A:272:ASN:N	1:A:272:ASN:HD22	2.07	0.51
1:B:367:LYS:HZ3	1:B:466:CYS:HA	1.75	0.51
1:C:44:ILE:HD11	1:C:61:ILE:HG21	1.92	0.51
1:E:437:THR:C	1:E:439:GLY:N	2.63	0.51
1:F:44:ILE:HD11	1:F:72:LEU:HD21	1.93	0.51
1:B:272:ASN:ND2	1:B:315:GLY:O	2.44	0.51
1:A:221:SER:HA	1:A:224:ILE:HD12	1.92	0.51
1:F:98:ILE:N	1:F:99:PRO:HD2	2.26	0.51
1:B:35:LEU:HD12	1:B:64:LEU:CD1	2.41	0.51
1:F:77:ARG:HE	1:F:80:VAL:HG23	1.75	0.51
1:C:17:ASP:HB3	1:C:20:MET:HE1	1.91	0.51
1:E:527:GLU:HG3	1:E:527:GLU:O	2.10	0.51
1:F:209:VAL:O	1:F:213:ILE:HB	2.10	0.51
1:F:139:THR:HG23	2:F:541:3NM:O1	2.11	0.51
1:D:55:ILE:HG23	1:D:84:ILE:CG2	2.39	0.51
1:A:192:TYR:HA	1:A:431:TYR:HB3	1.93	0.51
1:A:257:ILE:HD11	1:A:533:TRP:HH2	1.75	0.51
1:D:98:ILE:HD11	1:D:113:TRP:NE1	2.25	0.51
1:B:139:THR:HG23	2:B:541:3NM:O1	2.11	0.51
1:D:8:PHE:CE2	1:D:110:VAL:HB	2.45	0.51
1:A:347:THR:HG21	1:C:298:GLU:CG	2.41	0.51
1:A:319:PRO:O	1:A:322:MET:HB3	2.10	0.51
1:A:484:ASN:HD21	1:A:486:PHE:HB3	1.75	0.51
1:E:323:LEU:CD1	1:E:357:LEU:HD11	2.40	0.51
1:C:517:LEU:O	1:C:517:LEU:HD23	2.11	0.51
1:A:268:GLN:CD	1:A:302:LEU:HD23	2.31	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:165:ALA:HA	1:E:168:ARG:NH2	2.24	0.51
1:D:189:ARG:HG3	1:D:193:GLN:HE21	1.76	0.51
1:B:32:GLU:HA	1:B:64:LEU:HD11	1.92	0.51
1:D:78:ILE:HG21	1:D:96:MET:HE2	1.92	0.51
1:A:451:GLU:HG2	1:A:452:ALA:N	2.25	0.51
1:A:123:GLU:O	1:A:127:MET:HG3	2.10	0.51
1:A:41:LEU:HD11	1:A:73:ILE:HD11	1.93	0.51
1:B:339:PHE:HE1	1:B:357:LEU:HD23	1.76	0.51
1:F:182:LEU:HB3	1:F:187:ILE:HG13	1.92	0.51
1:C:286:LEU:HD21	1:C:521:LEU:HD22	1.93	0.51
1:E:18:SER:O	1:E:21:ILE:HG13	2.10	0.51
1:A:43:GLN:HA	1:A:73:ILE:O	2.11	0.51
1:A:268:GLN:HG2	1:A:310:LEU:CD1	2.41	0.51
1:D:484:ASN:HD21	1:D:486:PHE:HB3	1.76	0.51
1:B:16:THR:HG22	1:B:17:ASP:N	2.26	0.51
1:B:534:ALA:N	1:B:535:PRO:CD	2.74	0.51
1:D:399:ILE:CD1	1:D:421:PHE:CE2	2.94	0.51
1:F:282:VAL:HG21	1:F:467:SER:CB	2.41	0.51
1:C:533:TRP:HB3	1:C:535:PRO:HD2	1.92	0.50
1:E:295:ILE:HG22	1:E:298:GLU:H	1.75	0.50
1:F:268:GLN:HB3	1:F:310:LEU:CD1	2.37	0.50
1:F:419:PHE:HB3	1:F:421:PHE:CE2	2.47	0.50
1:F:305:ILE:HG23	1:F:306:PRO:HD2	1.92	0.50
1:C:275:HIS:N	1:C:275:HIS:CD2	2.78	0.50
1:D:272:ASN:O	1:D:276:GLN:HB2	2.11	0.50
1:D:151:LYS:O	1:D:152:ALA:CB	2.59	0.50
1:B:272:ASN:N	1:B:272:ASN:ND2	2.60	0.50
1:D:476:ILE:HD11	1:D:489:VAL:HG22	1.94	0.50
1:D:328:ARG:CG	1:D:328:ARG:HH11	2.25	0.50
1:B:184:PRO:HD3	1:B:211:ASP:OD1	2.11	0.50
1:A:280:ALA:HB2	1:A:292:MET:HE2	1.93	0.50
1:C:125:SER:HB2	1:C:169:ASN:HD22	1.74	0.50
1:F:475:MET:HE1	1:F:495:LEU:HD12	1.93	0.50
1:F:406:ALA:HB1	1:F:411:THR:O	2.11	0.50
1:A:299:VAL:CG2	1:A:326:ALA:HA	2.34	0.50
1:C:41:LEU:HD21	1:C:73:ILE:HD11	1.93	0.50
1:C:316:SER:O	1:C:317:VAL:HB	2.11	0.50
1:C:124:LEU:HD23	1:C:124:LEU:C	2.31	0.50
1:E:78:ILE:HG21	1:E:96:MET:CE	2.42	0.50
1:B:495:LEU:O	1:B:495:LEU:HD23	2.11	0.50
1:D:10:TYR:O	1:D:11:SER:C	2.50	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:257:ILE:HD13	1:D:525:THR:HG22	1.94	0.50
1:D:257:ILE:HG12	1:D:475:MET:HE1	1.94	0.50
1:E:179:ILE:HG13	1:E:207:CYS:SG	2.51	0.50
1:A:101:ILE:O	1:A:105:VAL:HG22	2.12	0.50
1:D:533:TRP:O	1:D:535:PRO:HD2	2.12	0.50
1:A:209:VAL:HG12	1:A:210:SER:N	2.26	0.50
1:A:298:GLU:HG3	1:B:347:THR:HG21	1.94	0.50
1:A:187:ILE:HG23	1:A:206:ILE:HD11	1.94	0.50
1:D:430:LYS:CD	1:D:437:THR:HG21	2.41	0.50
1:C:125:SER:C	1:C:127:MET:H	2.16	0.50
1:B:365:CYS:HA	1:B:412:VAL:O	2.12	0.50
1:B:75:ASN:O	1:B:77:ARG:N	2.38	0.49
1:C:276:GLN:HG3	1:C:292:MET:CE	2.42	0.49
1:C:73:ILE:HA	1:C:88:GLY:O	2.12	0.49
1:F:241:LEU:O	1:F:428:GLU:HA	2.12	0.49
1:C:188:GLU:HG3	1:C:228:LEU:HG	1.94	0.49
1:E:299:VAL:CG1	1:E:300:ASN:N	2.75	0.49
1:A:509:GLY:HA2	1:C:522:TYR:HD2	1.75	0.49
1:D:35:LEU:HD12	1:D:64:LEU:HD13	1.93	0.49
1:F:482:GLU:H	1:F:482:GLU:CD	2.16	0.49
1:D:192:TYR:CE2	1:D:410:LYS:HG3	2.47	0.49
1:B:209:VAL:HG21	2:B:541:3NM:H6A	1.94	0.49
1:D:283:THR:HG22	1:D:288:SER:HB2	1.92	0.49
1:E:192:TYR:HA	1:E:431:TYR:HB3	1.94	0.49
1:B:424:ASP:HB3	1:B:446:PRO:HG2	1.94	0.49
1:F:228:LEU:N	1:F:228:LEU:CD1	2.75	0.49
1:C:275:HIS:HD2	1:C:275:HIS:H	1.58	0.49
1:D:247:LEU:HD22	1:D:537:LEU:HG	1.95	0.49
1:A:437:THR:O	1:A:439:GLY:N	2.45	0.49
1:B:265:PRO:HB3	1:B:307:HIS:O	2.12	0.49
1:D:19:GLY:O	1:D:20:MET:HB2	2.12	0.49
1:C:144:LEU:HD12	1:C:144:LEU:N	2.09	0.49
1:D:347:THR:HG21	1:E:298:GLU:HG2	1.94	0.49
1:A:417:GLY:O	1:A:497:LYS:NZ	2.45	0.49
1:B:267:VAL:CG1	1:B:269:HIS:CE1	2.96	0.49
1:A:51:THR:HB	1:E:95:ASP:HA	1.94	0.49
1:B:495:LEU:HD22	1:B:521:LEU:CD2	2.38	0.49
1:F:171:ALA:HA	1:F:173:TRP:CZ3	2.48	0.49
1:C:76:ASP:HA	1:C:91:VAL:HG12	1.95	0.49
1:C:208:VAL:HG11	1:C:225:LEU:HD13	1.93	0.49
1:D:480:PRO:O	1:D:482:GLU:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:78:ILE:O	1:C:81:ALA:HB3	2.13	0.49
1:D:341:PRO:O	1:D:342:VAL:C	2.51	0.49
1:F:182:LEU:HD12	1:F:190:VAL:HG21	1.94	0.49
1:B:34:GLY:O	1:B:39:VAL:HG23	2.12	0.49
1:A:419:PHE:CE1	1:A:451:GLU:HB2	2.48	0.49
1:D:124:LEU:HD23	1:D:124:LEU:C	2.33	0.49
1:C:345:SER:HA	1:C:351:LEU:HD13	1.94	0.49
1:B:61:ILE:HG22	1:B:72:LEU:HD22	1.95	0.48
1:A:78:ILE:HD11	1:A:104:LEU:HD12	1.95	0.48
1:B:275:HIS:N	1:B:275:HIS:HD2	2.11	0.48
1:F:125:SER:O	1:F:127:MET:N	2.46	0.48
1:B:111:ILE:HG23	1:B:132:VAL:HA	1.94	0.48
1:A:274:VAL:HG11	1:C:292:MET:HG3	1.95	0.48
1:E:362:GLN:NE2	1:E:362:GLN:HA	2.28	0.48
1:C:472:ILE:HD13	1:C:489:VAL:HG13	1.95	0.48
1:A:77:ARG:HG2	1:A:77:ARG:NH1	2.27	0.48
1:E:73:ILE:N	1:E:73:ILE:HD12	2.27	0.48
1:C:109:MET:HG2	1:C:110:VAL:N	2.27	0.48
1:C:424:ASP:HB2	1:C:486:PHE:CD1	2.48	0.48
1:C:64:LEU:O	1:C:64:LEU:HD22	2.11	0.48
1:A:187:ILE:HG23	1:A:206:ILE:CD1	2.43	0.48
1:E:160:ILE:HD13	1:E:195:VAL:O	2.12	0.48
1:D:430:LYS:HD2	1:D:437:THR:HG21	1.94	0.48
1:C:226:ARG:HD3	1:C:226:ARG:HA	1.63	0.48
1:A:484:ASN:ND2	1:A:487:HIS:H	2.12	0.48
1:D:8:PHE:HD1	1:D:71:PRO:HG2	1.77	0.48
1:A:527:GLU:O	1:A:529:THR:N	2.46	0.48
1:F:411:THR:HA	1:F:426:THR:HG22	1.94	0.48
1:A:92:GLY:HA3	4:A:543:POP:O4	2.13	0.48
1:C:276:GLN:HG3	1:C:292:MET:HE3	1.96	0.48
1:D:110:VAL:HG23	1:D:133:ASP:HB2	1.94	0.48
1:F:512:SER:HA	1:F:515:VAL:HG12	1.95	0.48
1:A:97:PRO:O	1:A:101:ILE:HG13	2.14	0.48
1:A:65:CYS:O	1:A:68:HIS:N	2.47	0.48
1:D:215:SER:C	1:D:217:ASP:H	2.16	0.48
1:F:403:LYS:HE2	1:F:447:CYS:HB2	1.96	0.48
1:D:313:ASN:C	1:D:313:ASN:ND2	2.66	0.48
1:B:88:GLY:HA3	1:B:110:VAL:HG13	1.95	0.48
1:E:494:MET:O	1:E:495:LEU:C	2.52	0.48
1:E:265:PRO:O	1:E:288:SER:HB3	2.13	0.48
1:D:256:ILE:HG22	1:D:475:MET:HE1	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:ILE:HD11	1:B:86:ALA:HB2	1.95	0.48
1:F:466:CYS:O	1:F:466:CYS:SG	2.72	0.48
1:F:41:LEU:HD12	1:F:71:PRO:HD2	1.96	0.48
1:D:278:PHE:CE1	1:D:518:ILE:HD11	2.49	0.48
1:B:187:ILE:HG23	1:B:206:ILE:HD11	1.95	0.48
1:A:476:ILE:HD11	1:A:489:VAL:CG2	2.43	0.48
1:A:135:ILE:O	1:A:135:ILE:HG13	2.13	0.48
1:F:280:ALA:O	1:F:284:LEU:HD22	2.14	0.48
1:E:78:ILE:HD13	1:E:96:MET:CE	2.39	0.48
1:E:479:GLN:HA	1:E:480:PRO:HD3	1.59	0.48
1:E:192:TYR:CE1	1:E:410:LYS:HB3	2.49	0.48
1:E:58:ALA:CB	1:E:84:ILE:HD13	2.40	0.48
1:E:522:TYR:O	1:E:526:ARG:HD3	2.14	0.48
1:B:89:ILE:HD11	1:B:101:ILE:HG21	1.94	0.47
1:D:340:ASP:HA	1:D:341:PRO:HD3	1.67	0.47
1:F:299:VAL:HG21	1:F:326:ALA:CB	2.45	0.47
1:B:98:ILE:HD12	1:B:111:ILE:HD13	1.95	0.47
1:D:275:HIS:CD2	1:D:275:HIS:N	2.80	0.47
1:F:524:LEU:HA	1:F:524:LEU:HD12	1.65	0.47
1:E:484:ASN:ND2	1:E:487:HIS:H	2.11	0.47
1:F:335:ARG:NH1	1:F:336:PRO:HD3	2.30	0.47
1:A:422:ILE:CD1	1:A:493:VAL:HG21	2.44	0.47
1:C:197:SER:O	1:C:442:VAL:HG23	2.14	0.47
1:F:517:LEU:HD23	1:F:517:LEU:C	2.34	0.47
1:D:467:SER:HB2	1:D:496:TYR:HE1	1.79	0.47
1:C:41:LEU:HD21	1:C:73:ILE:CD1	2.44	0.47
1:B:224:ILE:O	1:B:228:LEU:HD13	2.13	0.47
1:C:272:ASN:ND2	1:C:272:ASN:N	2.62	0.47
1:D:370:SER:O	1:D:374:LEU:HB2	2.14	0.47
1:E:8:PHE:HE1	1:E:71:PRO:HB3	1.80	0.47
1:C:256:ILE:HD13	1:C:488:ALA:HA	1.97	0.47
1:A:357:LEU:O	1:A:360:PHE:HB2	2.14	0.47
1:A:116:GLY:C	1:A:117:PHE:HD2	2.16	0.47
1:D:253:ILE:O	1:D:257:ILE:HG13	2.13	0.47
1:C:472:ILE:O	1:C:476:ILE:HG13	2.14	0.47
1:D:295:ILE:HG22	1:D:298:GLU:H	1.80	0.47
1:C:135:ILE:CG1	1:C:176:THR:HG22	2.44	0.47
1:C:322:MET:HE3	1:C:326:ALA:HB2	1.96	0.47
1:E:79:ASP:OD1	1:E:80:VAL:HG23	2.15	0.47
1:E:191:LEU:HD12	1:E:191:LEU:HA	1.69	0.47
1:B:77:ARG:NH1	1:F:77:ARG:CZ	2.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:313:ASN:O	1:C:314:THR:C	2.53	0.47
1:C:3:PHE:CE2	1:C:71:PRO:HA	2.50	0.47
1:F:179:ILE:HG12	1:F:180:GLY:N	2.29	0.47
1:F:265:PRO:O	1:F:288:SER:HB3	2.14	0.47
1:C:189:ARG:O	1:C:193:GLN:HG2	2.14	0.47
1:E:442:VAL:O	1:E:445:ILE:HG12	2.14	0.47
1:E:166:LEU:CD2	1:E:171:ALA:HB3	2.44	0.47
1:B:78:ILE:HG12	1:B:79:ASP:N	2.29	0.47
1:E:299:VAL:HG13	1:E:300:ASN:N	2.28	0.47
1:D:344:TYR:C	1:D:346:ALA:H	2.18	0.47
1:F:75:ASN:O	1:F:77:ARG:N	2.39	0.47
1:D:91:VAL:HG11	1:D:101:ILE:CD1	2.44	0.47
1:F:247:LEU:HD22	1:F:537:LEU:HG	1.97	0.47
1:E:168:ARG:CZ	1:E:168:ARG:HB3	2.44	0.47
1:D:112:GLY:HA3	1:D:134:TYR:CE2	2.49	0.47
1:A:308:ALA:O	1:A:335:ARG:HD3	2.15	0.47
1:B:519:ASP:O	1:B:522:TYR:HB3	2.15	0.47
1:A:271:THR:HA	1:A:313:ASN:HB3	1.96	0.47
1:A:116:GLY:C	1:A:117:PHE:CD2	2.89	0.47
1:F:324:LYS:HA	1:F:360:PHE:CD1	2.50	0.47
1:F:283:THR:HG23	1:F:288:SER:HB2	1.97	0.47
1:A:308:ALA:O	1:A:335:ARG:NH1	2.41	0.47
1:B:370:SER:O	1:B:374:LEU:HB2	2.14	0.47
1:D:324:LYS:HB2	1:D:360:PHE:CE1	2.50	0.47
1:D:34:GLY:O	1:D:39:VAL:HG23	2.15	0.47
1:F:74:ILE:HD12	1:F:86:ALA:HB2	1.97	0.47
1:E:328:ARG:HG3	1:E:328:ARG:HH11	1.75	0.47
1:D:484:ASN:ND2	1:D:487:HIS:H	2.11	0.47
1:F:78:ILE:HB	1:F:89:ILE:HD12	1.96	0.47
1:D:299:VAL:CG1	1:D:300:ASN:N	2.78	0.47
1:A:187:ILE:HD13	1:A:225:LEU:HD22	1.96	0.47
1:C:275:HIS:HB3	1:C:466:CYS:SG	2.55	0.47
1:F:187:ILE:HG12	1:F:206:ILE:CD1	2.45	0.47
1:F:191:LEU:HD22	1:F:206:ILE:HD11	1.96	0.47
1:A:422:ILE:HD13	1:A:493:VAL:HG21	1.96	0.47
1:A:35:LEU:CD2	1:A:70:VAL:HG11	2.39	0.46
1:E:19:GLY:O	1:E:20:MET:CB	2.63	0.46
1:F:472:ILE:O	1:F:476:ILE:HG13	2.15	0.46
1:F:239:ILE:HG22	1:F:240:GLY:N	2.31	0.46
1:F:102:ARG:NH1	1:F:109:MET:O	2.38	0.46
1:C:206:ILE:HB	1:C:229:ILE:HD11	1.95	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:SER:N	1:A:7:GLN:OE1	2.47	0.46
1:E:335:ARG:HB3	1:E:336:PRO:CD	2.45	0.46
1:B:79:ASP:OD1	1:B:80:VAL:HG23	2.14	0.46
1:A:96:MET:HE3	1:A:101:ILE:HG12	1.96	0.46
1:F:193:GLN:NE2	1:F:362:GLN:NE2	2.63	0.46
1:E:20:MET:HE2	1:E:213:ILE:HG21	1.97	0.46
1:A:316:SER:C	1:A:317:VAL:HG23	2.36	0.46
1:E:260:THR:HA	1:E:478:GLY:HA3	1.97	0.46
1:E:41:LEU:HD11	1:E:73:ILE:CD1	2.42	0.46
1:B:191:LEU:HA	1:B:191:LEU:HD12	1.68	0.46
2:A:541:3NM:N	3:A:542:IFP:C7A	2.79	0.46
1:A:433:LEU:CD1	1:A:433:LEU:N	2.78	0.46
1:F:406:ALA:HB2	1:F:413:ALA:HB3	1.98	0.46
1:F:338:VAL:HG22	1:F:365:CYS:HB3	1.97	0.46
1:A:159:ALA:O	1:A:162:VAL:HB	2.16	0.46
1:E:399:ILE:HD11	1:E:421:PHE:CE2	2.50	0.46
1:A:191:LEU:HA	1:A:191:LEU:HD12	1.66	0.46
1:C:302:LEU:HD13	1:C:302:LEU:H	1.80	0.46
1:D:416:THR:HG22	1:D:420:ASP:OD1	2.16	0.46
1:A:534:ALA:H	1:A:535:PRO:CD	2.27	0.46
1:E:10:TYR:O	1:E:205:GLY:HA3	2.15	0.46
1:C:479:GLN:HA	1:C:480:PRO:HD3	1.66	0.46
1:A:8:PHE:CD1	1:A:71:PRO:HG2	2.50	0.46
1:E:8:PHE:CZ	1:E:110:VAL:HG11	2.50	0.46
1:D:283:THR:CG2	1:D:288:SER:HB2	2.46	0.46
1:C:339:PHE:HE2	1:C:341:PRO:HG3	1.78	0.46
1:E:28:TYR:CE1	1:E:64:LEU:HG	2.51	0.46
1:A:298:GLU:HG2	1:A:302:LEU:HD13	1.98	0.46
1:B:422:ILE:CG2	1:B:486:PHE:HE1	2.28	0.46
1:E:73:ILE:HG22	1:E:74:ILE:N	2.31	0.46
1:B:240:GLY:C	1:B:241:LEU:HG	2.35	0.46
1:C:129:PRO:HG3	1:C:173:TRP:CD2	2.50	0.46
1:E:312:LEU:HA	1:E:312:LEU:HD13	1.62	0.46
1:A:268:GLN:OE1	1:A:302:LEU:HD23	2.16	0.46
1:F:8:PHE:CD1	1:F:71:PRO:HG2	2.51	0.46
1:C:264:ARG:N	1:C:265:PRO:CD	2.78	0.46
1:E:296:GLN:HG2	1:E:322:MET:HB2	1.96	0.46
1:B:427:ILE:O	1:B:429:GLY:N	2.49	0.46
1:A:142:PRO:HA	1:A:153:PRO:HG3	1.98	0.46
1:A:298:GLU:OE1	1:B:350:ARG:HD2	2.16	0.46
1:D:299:VAL:HG21	1:D:326:ALA:CA	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:437:THR:C	1:F:439:GLY:N	2.65	0.46
1:B:209:VAL:O	1:B:213:ILE:HG12	2.16	0.46
1:E:125:SER:O	1:E:127:MET:N	2.49	0.46
1:A:407:PHE:CD1	1:A:442:VAL:HG22	2.51	0.46
1:E:66:HIS:HE1	1:E:87:ASP:OD1	1.99	0.46
1:A:394:SER:OG	1:A:395:ASN:N	2.49	0.46
1:A:77:ARG:HH12	1:E:77:ARG:CG	2.29	0.46
1:D:78:ILE:HG13	1:D:79:ASP:N	2.24	0.46
1:A:192:TYR:HD2	1:A:192:TYR:O	1.99	0.46
1:D:278:PHE:HE1	1:D:518:ILE:HD11	1.80	0.46
1:A:115:VAL:HA	1:A:120:GLU:OE1	2.16	0.46
1:C:65:CYS:HB3	1:C:70:VAL:O	2.16	0.46
1:C:322:MET:HG3	1:C:323:LEU:N	2.28	0.45
1:B:422:ILE:N	1:B:422:ILE:HD12	2.31	0.45
1:B:484:ASN:HD21	1:B:486:PHE:HB3	1.81	0.45
1:D:89:ILE:HD12	1:D:91:VAL:HG13	1.98	0.45
1:C:183:HIS:C	1:C:187:ILE:HD12	2.36	0.45
1:C:298:GLU:HG2	1:C:302:LEU:CD1	2.44	0.45
1:A:509:GLY:CA	1:C:522:TYR:HD2	2.29	0.45
1:A:280:ALA:O	1:A:284:LEU:HD22	2.16	0.45
1:E:98:ILE:N	1:E:99:PRO:CD	2.78	0.45
1:D:115:VAL:HG13	1:D:120:GLU:HB3	1.98	0.45
1:F:450:VAL:HG21	1:F:494:MET:HG2	1.96	0.45
1:E:86:ALA:O	1:E:109:MET:CE	2.64	0.45
1:A:55:ILE:HG23	1:A:84:ILE:HG21	1.99	0.45
1:F:373:ILE:HG13	1:F:415:CYS:CB	2.45	0.45
1:D:298:GLU:CG	1:F:347:THR:HG21	2.43	0.45
1:C:119:GLU:O	1:C:122:ASP:HB2	2.16	0.45
1:E:30:GLN:OE1	1:E:30:GLN:HA	2.15	0.45
1:E:88:GLY:HA3	1:E:110:VAL:HG13	1.98	0.45
1:E:8:PHE:CD1	1:E:71:PRO:HG2	2.52	0.45
1:B:70:VAL:HG23	1:B:71:PRO:HD2	1.98	0.45
1:F:529:THR:O	1:F:532:THR:HG23	2.17	0.45
1:A:113:TRP:HB3	1:A:135:ILE:HG22	1.98	0.45
1:F:329:ALA:O	1:F:333:VAL:HG23	2.16	0.45
1:B:59:LEU:O	1:B:60:GLN:C	2.53	0.45
1:A:495:LEU:HD22	1:A:521:LEU:HD23	1.98	0.45
1:D:369:ASN:O	1:D:370:SER:C	2.54	0.45
1:D:136:GLY:HA2	1:D:177:VAL:HG23	1.99	0.45
1:F:226:ARG:HA	1:F:226:ARG:HD3	1.77	0.45
1:B:118:PRO:HA	1:B:121:VAL:HG23	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:109:MET:CG	1:F:110:VAL:N	2.79	0.45
1:D:192:TYR:HD2	1:D:192:TYR:O	2.00	0.45
1:D:276:GLN:CG	1:D:292:MET:HE2	2.38	0.45
1:C:328:ARG:CG	1:C:328:ARG:NH1	2.73	0.45
1:E:186:ASN:C	1:E:186:ASN:ND2	2.62	0.45
1:D:399:ILE:CD1	1:D:421:PHE:CD2	3.00	0.45
1:F:224:ILE:O	1:F:228:LEU:HD13	2.17	0.45
1:B:339:PHE:CD2	1:B:341:PRO:HG3	2.52	0.45
1:E:182:LEU:HD12	1:E:190:VAL:HG21	1.99	0.45
1:A:328:ARG:NH1	1:A:328:ARG:CG	2.74	0.45
1:E:437:THR:O	1:E:438:ASN:C	2.54	0.45
1:D:10:TYR:O	1:D:205:GLY:HA3	2.17	0.45
1:B:427:ILE:C	1:B:429:GLY:H	2.20	0.45
1:F:226:ARG:O	1:F:227:GLY:C	2.55	0.45
1:D:102:ARG:NH1	1:D:109:MET:O	2.47	0.45
1:A:212:ILE:O	1:A:215:SER:HB3	2.17	0.45
1:E:55:ILE:HG23	1:E:84:ILE:HG22	1.99	0.45
1:F:64:LEU:O	1:F:64:LEU:HD22	2.16	0.45
1:F:15:VAL:HG22	1:F:43:GLN:HE21	1.81	0.45
1:D:344:TYR:O	1:D:350:ARG:HB3	2.17	0.45
1:C:530:PRO:HA	1:C:533:TRP:CE2	2.52	0.45
1:E:115:VAL:HG13	1:E:120:GLU:CB	2.45	0.45
1:A:4:SER:O	1:A:5:LYS:C	2.55	0.45
1:A:189:ARG:NH1	1:A:359:THR:O	2.50	0.45
1:C:433:LEU:O	1:C:434:SER:CB	2.65	0.45
1:D:338:VAL:HG21	1:D:473:ALA:HB2	1.99	0.45
1:D:524:LEU:HD12	1:D:524:LEU:HA	1.65	0.45
1:A:313:ASN:HD22	1:A:342:VAL:HG21	1.72	0.45
1:C:225:LEU:O	1:C:229:ILE:HG13	2.17	0.45
1:D:274:VAL:HG13	1:E:276:GLN:HG2	1.98	0.45
1:B:14:LEU:HD11	1:B:213:ILE:CD1	2.44	0.45
1:E:484:ASN:HD21	1:E:486:PHE:HB3	1.82	0.45
1:B:125:SER:C	1:B:127:MET:N	2.71	0.45
1:D:11:SER:CB	1:D:226:ARG:HH12	2.30	0.45
1:E:166:LEU:HD22	1:E:171:ALA:HB3	1.99	0.45
1:D:179:ILE:HG13	1:D:207:CYS:SG	2.57	0.45
1:C:97:PRO:O	1:C:101:ILE:HG13	2.17	0.45
1:E:8:PHE:HE1	1:E:71:PRO:CB	2.30	0.45
1:A:416:THR:HG22	1:A:420:ASP:OD1	2.17	0.45
1:C:74:ILE:HD11	1:C:84:ILE:HD11	1.99	0.45
1:E:534:ALA:N	1:E:535:PRO:HD3	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:394:SER:OG	1:B:395:ASN:N	2.48	0.45
1:E:509:GLY:HA3	1:F:519:ASP:OD1	2.17	0.45
1:C:169:ASN:O	1:C:170:ASN:C	2.56	0.44
1:B:239:ILE:HG22	1:B:240:GLY:N	2.32	0.44
1:F:231:LYS:HG2	1:F:232:THR:H	1.82	0.44
1:C:347:THR:OG1	1:C:350:ARG:HB2	2.18	0.44
1:A:280:ALA:O	1:A:284:LEU:CD2	2.66	0.44
1:B:328:ARG:CG	1:B:328:ARG:NH1	2.74	0.44
1:C:193:GLN:NE2	1:C:362:GLN:HE21	2.15	0.44
1:F:357:LEU:HA	1:F:357:LEU:HD13	1.67	0.44
1:E:485:LEU:O	1:E:489:VAL:HG23	2.17	0.44
1:D:305:ILE:H	1:D:305:ILE:HG13	1.59	0.44
1:A:274:VAL:HG11	1:C:292:MET:CG	2.48	0.44
1:B:27:LEU:HD23	1:B:57:GLU:OE1	2.16	0.44
1:C:109:MET:CG	1:C:110:VAL:N	2.80	0.44
1:D:121:VAL:CG1	1:D:166:LEU:HD23	2.47	0.44
1:C:355:ASN:O	1:C:359:THR:HG23	2.16	0.44
1:A:295:ILE:N	1:A:295:ILE:HD12	2.32	0.44
1:A:183:HIS:HB3	1:A:184:PRO:CD	2.48	0.44
1:D:512:SER:HA	1:D:515:VAL:CG1	2.40	0.44
1:F:193:GLN:NE2	1:F:362:GLN:HE21	2.16	0.44
1:E:19:GLY:O	1:E:20:MET:HB2	2.17	0.44
1:C:237:VAL:HA	1:C:334:LYS:O	2.17	0.44
1:A:224:ILE:O	1:A:228:LEU:HD13	2.18	0.44
1:A:59:LEU:CD2	1:A:84:ILE:HB	2.47	0.44
1:C:322:MET:CE	1:C:326:ALA:HB2	2.48	0.44
1:F:253:ILE:O	1:F:257:ILE:HG13	2.18	0.44
1:B:524:LEU:HD12	1:B:524:LEU:HA	1.79	0.44
1:C:59:LEU:HD21	1:C:84:ILE:HB	1.99	0.44
1:E:407:PHE:HE2	1:E:427:ILE:CD1	2.30	0.44
1:C:129:PRO:HG3	1:C:173:TRP:CE3	2.52	0.44
1:C:80:VAL:O	1:C:83:ALA:HB3	2.18	0.44
1:D:224:ILE:O	1:D:228:LEU:HD13	2.18	0.44
1:A:183:HIS:HB3	1:A:184:PRO:HD2	1.99	0.44
1:B:77:ARG:NH1	1:B:77:ARG:HG2	2.29	0.44
1:E:267:VAL:CG1	1:E:269:HIS:CE1	3.00	0.44
1:A:369:ASN:O	1:A:370:SER:C	2.56	0.44
1:A:468:LEU:O	1:A:468:LEU:HD12	2.18	0.44
1:E:468:LEU:HD12	1:E:472:ILE:HG13	2.00	0.44
1:C:427:ILE:C	1:C:429:GLY:H	2.20	0.44
1:E:283:THR:HB	1:E:290:PRO:HG3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:278:PHE:CE2	1:F:467:SER:OG	2.70	0.44
1:C:299:VAL:CG2	1:C:326:ALA:HA	2.34	0.44
1:F:523:ARG:O	1:F:527:GLU:HG2	2.18	0.44
1:F:403:LYS:HE2	1:F:447:CYS:CB	2.48	0.44
1:B:369:ASN:O	1:B:370:SER:C	2.56	0.44
1:E:422:ILE:HD12	1:E:490:VAL:HG22	1.99	0.44
1:F:112:GLY:HA3	1:F:134:TYR:CZ	2.52	0.44
1:E:237:VAL:HA	1:E:334:LYS:O	2.18	0.44
1:D:119:GLU:CD	1:D:119:GLU:H	2.21	0.44
1:B:352:LEU:HD22	1:B:352:LEU:HA	1.54	0.44
1:E:55:ILE:HG23	1:E:84:ILE:CG2	2.47	0.44
1:C:339:PHE:CD2	1:C:341:PRO:HG3	2.53	0.44
1:A:437:THR:C	1:A:439:GLY:N	2.71	0.44
1:E:187:ILE:HG23	1:E:206:ILE:HD13	2.00	0.44
1:A:256:ILE:HD13	1:A:488:ALA:HA	2.00	0.44
1:F:437:THR:O	1:F:438:ASN:C	2.56	0.44
1:C:341:PRO:HB3	1:C:354:ASN:OD1	2.17	0.44
1:F:182:LEU:CD1	1:F:190:VAL:HG21	2.48	0.44
1:D:5:LYS:HE2	1:D:133:ASP:OD2	2.17	0.44
1:C:534:ALA:N	1:C:535:PRO:CD	2.80	0.44
1:B:256:ILE:HD13	1:B:488:ALA:HA	2.00	0.44
1:C:394:SER:HB3	1:C:397:LEU:HB3	1.98	0.44
1:A:228:LEU:N	1:A:228:LEU:CD1	2.81	0.44
1:B:93:GLN:OE1	1:B:120:GLU:HG2	2.18	0.43
1:D:272:ASN:N	1:D:272:ASN:HD22	2.16	0.43
1:D:368:GLY:O	1:D:415:CYS:HA	2.18	0.43
1:C:495:LEU:HA	1:C:495:LEU:HD23	1.83	0.43
1:F:495:LEU:O	1:F:495:LEU:HD23	2.17	0.43
1:F:260:THR:HA	1:F:478:GLY:HA3	2.00	0.43
1:C:500:GLY:O	1:C:504:SER:HB3	2.18	0.43
1:A:524:LEU:HD12	1:A:524:LEU:HA	1.75	0.43
1:A:35:LEU:CD1	1:A:64:LEU:HD13	2.46	0.43
1:A:339:PHE:HE2	1:A:341:PRO:HG3	1.72	0.43
1:B:266:LEU:HD23	1:B:305:ILE:CG2	2.45	0.43
1:D:373:ILE:HD13	1:D:373:ILE:HA	1.78	0.43
1:F:115:VAL:O	1:F:138:GLY:N	2.44	0.43
1:B:19:GLY:O	1:B:20:MET:HB2	2.17	0.43
1:C:257:ILE:HD11	1:C:533:TRP:HH2	1.83	0.43
1:F:495:LEU:CD2	1:F:521:LEU:HD23	2.48	0.43
1:E:452:ALA:HB2	1:E:535:PRO:HB3	2.00	0.43
1:E:4:SER:O	1:E:5:LYS:C	2.57	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:316:SER:C	1:F:318:ALA:H	2.20	0.43
1:C:445:ILE:O	1:C:445:ILE:HG13	2.17	0.43
1:A:73:ILE:HG23	1:A:88:GLY:O	2.18	0.43
1:E:274:VAL:HG13	1:F:276:GLN:HG2	2.00	0.43
1:F:32:GLU:HA	1:F:64:LEU:HD11	2.00	0.43
1:A:432:SER:C	1:A:433:LEU:HD12	2.39	0.43
1:D:115:VAL:HG13	1:D:120:GLU:HB2	2.00	0.43
1:A:124:LEU:HD23	1:A:124:LEU:C	2.39	0.43
1:F:171:ALA:O	1:F:173:TRP:N	2.51	0.43
1:B:237:VAL:HA	1:B:334:LYS:O	2.19	0.43
1:C:98:ILE:N	1:C:99:PRO:HD2	2.33	0.43
1:B:133:ASP:O	1:B:174:CYS:HA	2.18	0.43
1:B:280:ALA:O	1:B:284:LEU:HD22	2.16	0.43
1:C:144:LEU:CD1	1:C:144:LEU:H	2.13	0.43
1:D:281:ASN:CB	1:D:518:ILE:HD13	2.43	0.43
1:D:3:PHE:CD2	1:D:71:PRO:HG3	2.52	0.43
1:B:125:SER:O	1:B:127:MET:N	2.51	0.43
1:C:402:THR:HG22	1:C:423:ALA:CB	2.49	0.43
3:B:542:IFP:H7A1	4:B:543:POP:O	2.18	0.43
1:F:110:VAL:CG1	1:F:111:ILE:N	2.82	0.43
1:F:271:THR:CA	1:F:313:ASN:HB3	2.43	0.43
1:F:124:LEU:HD23	1:F:125:SER:N	2.33	0.43
1:F:16:THR:CG2	1:F:17:ASP:N	2.80	0.43
1:C:228:LEU:HA	1:C:228:LEU:HD12	1.84	0.43
1:D:15:VAL:HG22	1:D:43:GLN:HB3	2.00	0.43
1:C:399:ILE:HD11	1:C:421:PHE:CE2	2.53	0.43
1:C:183:HIS:HB3	1:C:184:PRO:CD	2.48	0.43
1:C:318:ALA:HA	1:C:319:PRO:HD3	1.84	0.43
1:E:125:SER:C	1:E:127:MET:N	2.67	0.43
1:A:296:GLN:HG3	1:A:322:MET:HA	1.99	0.43
1:E:264:ARG:N	1:E:265:PRO:HD3	2.34	0.43
1:C:59:LEU:CD2	1:C:84:ILE:HB	2.48	0.43
1:A:140:LEU:HB3	1:A:141:PHE:CD2	2.53	0.43
1:F:78:ILE:O	1:F:82:MET:HG3	2.18	0.43
1:B:347:THR:OG1	1:B:350:ARG:HB2	2.18	0.43
1:F:8:PHE:CD2	1:F:110:VAL:HG21	2.45	0.43
1:B:298:GLU:OE1	1:C:350:ARG:HD2	2.18	0.43
1:E:182:LEU:HA	1:E:186:ASN:HD21	1.83	0.43
1:E:98:ILE:H	1:E:99:PRO:HD2	1.80	0.43
1:F:335:ARG:CZ	1:F:336:PRO:HD3	2.48	0.43
1:F:475:MET:HE2	1:F:495:LEU:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:160:ILE:HD11	1:C:193:GLN:O	2.19	0.43
1:B:479:GLN:HA	1:B:480:PRO:HD3	1.64	0.43
1:C:208:VAL:HG11	1:C:225:LEU:CD1	2.49	0.43
1:D:322:MET:HG3	1:D:323:LEU:N	2.33	0.43
1:E:335:ARG:HB3	1:E:336:PRO:HD3	2.00	0.43
1:B:74:ILE:HD12	1:B:81:ALA:HA	2.00	0.43
1:C:151:LYS:HB3	1:C:152:ALA:H	1.63	0.43
1:E:368:GLY:O	1:E:415:CYS:HA	2.19	0.43
1:B:96:MET:O	1:B:97:PRO:C	2.55	0.43
1:F:110:VAL:HG13	1:F:133:ASP:HB2	2.01	0.43
1:D:206:ILE:HB	1:D:229:ILE:HD11	2.00	0.43
1:B:341:PRO:O	1:B:372:GLU:HG2	2.19	0.43
1:D:78:ILE:O	1:D:82:MET:HG3	2.18	0.43
1:C:191:LEU:HD22	1:C:206:ILE:HD11	1.99	0.43
1:B:98:ILE:HD13	1:B:98:ILE:HA	1.72	0.43
1:F:295:ILE:HD12	1:F:295:ILE:N	2.33	0.43
1:D:395:ASN:HA	1:D:398:LEU:HD12	1.99	0.43
1:C:17:ASP:HB3	1:C:20:MET:HE2	2.01	0.43
1:E:31:VAL:O	1:E:31:VAL:HG12	2.19	0.43
1:C:348:GLU:OE1	1:C:348:GLU:HA	2.19	0.43
1:C:101:ILE:O	1:C:105:VAL:CG2	2.66	0.42
1:A:78:ILE:CD1	1:A:104:LEU:HD12	2.49	0.42
1:A:65:CYS:HB3	1:A:70:VAL:O	2.19	0.42
1:D:187:ILE:HG23	1:D:206:ILE:HD12	2.00	0.42
1:C:17:ASP:CB	1:C:20:MET:HE1	2.48	0.42
1:C:451:GLU:HG2	1:C:452:ALA:N	2.34	0.42
1:B:228:LEU:N	1:B:228:LEU:HD12	2.34	0.42
1:A:16:THR:HB	1:A:44:ILE:HA	2.01	0.42
1:F:266:LEU:HD23	1:F:305:ILE:HG21	2.00	0.42
1:E:344:TYR:C	1:E:346:ALA:H	2.22	0.42
1:D:255:SER:O	1:D:259:ASN:ND2	2.52	0.42
1:E:253:ILE:O	1:E:257:ILE:HG13	2.18	0.42
1:B:138:GLY:HA3	1:B:154:MET:HE2	2.01	0.42
1:D:80:VAL:O	1:D:84:ILE:HG12	2.19	0.42
1:A:192:TYR:CD1	1:A:234:TYR:CD2	3.01	0.42
1:F:121:VAL:O	1:F:124:LEU:CD2	2.67	0.42
1:A:256:ILE:HG12	1:A:479:GLN:OE1	2.19	0.42
1:C:437:THR:C	1:C:439:GLY:H	2.21	0.42
1:B:305:ILE:HA	1:B:306:PRO:HD3	1.87	0.42
1:F:479:GLN:HA	1:F:480:PRO:HD3	1.66	0.42
1:D:88:GLY:HA3	1:D:110:VAL:HG13	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:402:THR:HG22	1:C:423:ALA:HB2	2.00	0.42
1:A:140:LEU:HD23	1:A:182:LEU:HD11	2.01	0.42
1:C:10:TYR:O	1:C:205:GLY:HA3	2.19	0.42
1:B:402:THR:OG1	1:B:415:CYS:HB2	2.20	0.42
1:A:241:LEU:O	1:A:428:GLU:HA	2.18	0.42
1:F:141:PHE:HB3	1:F:142:PRO:CD	2.49	0.42
1:C:16:THR:O	1:C:45:ARG:HB3	2.19	0.42
1:D:427:ILE:C	1:D:429:GLY:H	2.21	0.42
1:E:450:VAL:O	1:E:450:VAL:HG12	2.20	0.42
1:A:313:ASN:ND2	1:A:342:VAL:HG22	2.31	0.42
1:B:414:VAL:HG22	1:B:422:ILE:HG13	2.02	0.42
1:E:101:ILE:O	1:E:105:VAL:CG2	2.59	0.42
1:B:323:LEU:HD12	1:B:357:LEU:HD11	2.02	0.42
1:B:276:GLN:OE1	1:C:273:LYS:CB	2.67	0.42
1:B:310:LEU:HD23	1:B:337:ILE:CG2	2.47	0.42
1:E:270:ILE:HD12	1:E:310:LEU:HD11	2.01	0.42
1:A:193:GLN:NE2	1:A:362:GLN:HE21	2.17	0.42
1:F:97:PRO:HG2	1:F:100:MET:HE3	2.01	0.42
1:D:234:TYR:HB2	1:D:431:TYR:CE1	2.54	0.42
1:F:35:LEU:CD2	1:F:70:VAL:HG11	2.40	0.42
1:D:98:ILE:N	1:D:99:PRO:HD2	2.35	0.42
1:A:139:THR:HG23	2:A:541:3NM:O1	2.19	0.42
1:A:322:MET:HG3	1:A:323:LEU:N	2.34	0.42
1:E:289:SER:HA	1:E:290:PRO:HD3	1.76	0.42
1:C:272:ASN:ND2	1:C:315:GLY:O	2.53	0.42
1:C:176:THR:O	1:C:204:ASP:HB2	2.19	0.42
1:B:333:VAL:O	1:B:334:LYS:HB2	2.20	0.42
1:B:45:ARG:NH2	4:B:543:POP:O1	2.40	0.42
1:A:314:THR:HG21	1:A:354:ASN:HD21	1.84	0.42
1:D:183:HIS:HB2	1:D:185:ASP:OD1	2.19	0.42
1:E:39:VAL:HG12	1:E:41:LEU:H	1.85	0.42
1:D:350:ARG:HD2	1:E:298:GLU:OE1	2.20	0.42
1:A:253:ILE:CD1	1:A:494:MET:CE	2.95	0.42
1:A:358:LEU:HD23	1:A:363:PHE:CE1	2.53	0.42
1:F:193:GLN:HE21	1:F:362:GLN:HE21	1.65	0.42
1:D:73:ILE:HA	1:D:88:GLY:O	2.18	0.42
1:C:257:ILE:HA	1:C:260:THR:HG22	2.01	0.42
1:E:117:PHE:N	1:E:117:PHE:CD2	2.85	0.42
1:A:534:ALA:H	1:A:535:PRO:HD3	1.84	0.42
1:C:115:VAL:HG13	1:C:120:GLU:CB	2.50	0.42
1:D:217:ASP:OD1	1:D:219:ALA:HB3	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:534:ALA:N	1:E:535:PRO:CD	2.83	0.42
1:F:318:ALA:HA	1:F:319:PRO:HD3	1.87	0.42
1:F:340:ASP:HA	1:F:341:PRO:HD3	1.76	0.42
1:F:59:LEU:HD21	1:F:84:ILE:CG2	2.49	0.42
1:F:123:GLU:O	1:F:127:MET:HG3	2.19	0.42
1:A:512:SER:HA	1:A:515:VAL:CG1	2.49	0.42
1:E:168:ARG:O	1:E:168:ARG:CG	2.68	0.42
1:E:248:THR:HG23	1:E:487:HIS:ND1	2.35	0.42
1:E:15:VAL:HB	1:E:209:VAL:CG2	2.49	0.42
1:C:335:ARG:HB3	1:C:336:PRO:CD	2.50	0.42
1:C:124:LEU:HD11	1:C:174:CYS:SG	2.60	0.42
1:E:16:THR:CG2	1:E:17:ASP:N	2.83	0.42
1:D:355:ASN:O	1:D:359:THR:HG23	2.20	0.42
1:C:77:ARG:NH2	1:D:77:ARG:HH12	2.17	0.42
1:F:124:LEU:HA	1:F:127:MET:HE3	1.99	0.42
1:C:495:LEU:HD11	1:C:525:THR:HG22	2.01	0.42
1:B:276:GLN:HG3	1:B:292:MET:HE2	2.01	0.42
1:E:144:LEU:HD12	1:E:144:LEU:N	2.34	0.42
1:D:21:ILE:HA	1:D:22:PRO:HD3	1.81	0.42
1:F:112:GLY:HA3	1:F:134:TYR:CE2	2.55	0.42
1:A:336:PRO:HA	1:A:364:SER:OG	2.19	0.42
1:C:406:ALA:HB2	1:C:413:ALA:HB3	2.01	0.42
1:E:175:ARG:HA	1:E:175:ARG:NE	2.34	0.42
1:B:73:ILE:HG23	1:B:89:ILE:HA	2.01	0.42
1:D:314:THR:HG21	1:D:354:ASN:HD21	1.85	0.42
1:B:326:ALA:O	1:B:329:ALA:HB3	2.20	0.42
1:F:533:TRP:HB3	1:F:535:PRO:HD2	2.01	0.42
1:F:16:THR:HG23	1:F:17:ASP:N	2.34	0.42
1:E:163:LEU:HD22	1:E:201:ARG:CD	2.50	0.42
1:D:253:ILE:HD11	1:D:494:MET:HE2	2.02	0.42
1:F:228:LEU:N	1:F:228:LEU:HD12	2.35	0.42
1:D:34:GLY:O	1:D:39:VAL:N	2.50	0.42
1:B:239:ILE:HG22	1:B:240:GLY:H	1.84	0.42
1:A:21:ILE:HA	1:A:22:PRO:HD3	1.60	0.42
1:C:270:ILE:HD12	1:C:310:LEU:HD11	2.02	0.42
1:D:353:LEU:O	1:D:357:LEU:HD13	2.20	0.42
1:A:102:ARG:HA	1:A:102:ARG:HD3	1.68	0.42
1:F:28:TYR:CZ	1:F:64:LEU:HG	2.55	0.42
1:B:192:TYR:CZ	1:B:410:LYS:HB3	2.54	0.42
1:D:44:ILE:CD1	1:D:58:ALA:HA	2.50	0.42
1:A:247:LEU:HA	1:A:247:LEU:HD23	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:524:LEU:HA	1:C:524:LEU:HD12	1.84	0.42
1:B:437:THR:O	1:B:439:GLY:N	2.53	0.42
1:E:179:ILE:HD12	3:E:542:IFP:C2A	2.50	0.42
1:A:523:ARG:HD3	1:B:508:ASN:O	2.19	0.42
1:C:322:MET:HG3	1:C:323:LEU:HD23	2.01	0.41
1:F:527:GLU:O	1:F:529:THR:N	2.53	0.41
1:E:138:GLY:HA3	1:E:154:MET:CE	2.50	0.41
1:E:15:VAL:HG22	1:E:43:GLN:HB3	2.01	0.41
1:B:468:LEU:HG	1:B:472:ILE:HD11	2.02	0.41
1:E:433:LEU:O	1:E:434:SER:CB	2.68	0.41
1:A:89:ILE:HD11	1:A:101:ILE:HG23	2.00	0.41
1:B:28:TYR:CE1	1:B:64:LEU:CG	3.01	0.41
1:C:72:LEU:N	1:C:87:ASP:OD1	2.53	0.41
1:E:416:THR:HA	1:E:420:ASP:OD1	2.21	0.41
1:D:352:LEU:HA	1:D:352:LEU:HD22	1.72	0.41
1:A:70:VAL:HG23	1:A:71:PRO:HD2	2.02	0.41
1:D:269:HIS:HB2	1:D:292:MET:CE	2.51	0.41
1:E:189:ARG:O	1:E:193:GLN:HG3	2.20	0.41
1:E:73:ILE:H	1:E:73:ILE:HD12	1.85	0.41
1:D:88:GLY:HA3	1:D:110:VAL:CG1	2.50	0.41
1:B:428:GLU:HG3	1:B:430:LYS:NZ	2.33	0.41
1:B:37:ASN:HD22	1:B:219:ALA:HA	1.85	0.41
1:D:527:GLU:O	1:D:527:GLU:HG3	2.19	0.41
1:B:257:ILE:O	1:B:257:ILE:HG22	2.20	0.41
1:F:247:LEU:CD2	1:F:537:LEU:HG	2.49	0.41
1:E:347:THR:HG21	1:F:298:GLU:CG	2.49	0.41
1:C:20:MET:HE3	1:C:213:ILE:HB	2.01	0.41
1:D:253:ILE:HD11	1:D:494:MET:CE	2.50	0.41
1:F:399:ILE:HG12	1:F:421:PHE:CD1	2.54	0.41
1:E:143:THR:HG21	2:E:541:3NM:H7	2.02	0.41
1:D:479:GLN:HA	1:D:480:PRO:HD3	1.73	0.41
1:A:501:LYS:O	1:A:504:SER:N	2.54	0.41
1:A:276:GLN:OE1	1:B:273:LYS:CB	2.69	0.41
1:D:141:PHE:HB3	1:D:142:PRO:CD	2.51	0.41
1:B:78:ILE:HD12	1:B:101:ILE:HG23	2.03	0.41
1:F:98:ILE:HG21	1:F:132:VAL:HG22	2.02	0.41
1:A:78:ILE:O	1:A:82:MET:HG3	2.20	0.41
1:F:59:LEU:HA	1:F:59:LEU:HD23	1.75	0.41
1:A:323:LEU:HD12	1:A:357:LEU:HD11	2.02	0.41
1:C:73:ILE:HG22	1:C:74:ILE:N	2.36	0.41
1:D:247:LEU:HD23	1:D:247:LEU:HA	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:318:ALA:HA	1:D:319:PRO:HD3	1.87	0.41
1:A:226:ARG:HA	1:A:226:ARG:HD3	1.69	0.41
1:C:89:ILE:HD11	1:C:101:ILE:HG21	2.02	0.41
1:D:78:ILE:HG21	1:D:96:MET:HE1	2.01	0.41
1:B:98:ILE:N	1:B:99:PRO:HD2	2.36	0.41
1:C:313:ASN:O	1:C:314:THR:O	2.38	0.41
1:E:175:ARG:HE	1:E:175:ARG:HA	1.85	0.41
1:C:192:TYR:CD1	1:C:234:TYR:HD2	2.38	0.41
1:C:77:ARG:NH2	1:D:77:ARG:NH1	2.69	0.41
1:A:350:ARG:O	1:A:351:LEU:C	2.57	0.41
1:D:192:TYR:C	1:D:192:TYR:CD2	2.93	0.41
1:D:206:ILE:HB	1:D:229:ILE:CD1	2.50	0.41
1:E:275:HIS:N	1:E:275:HIS:CD2	2.89	0.41
1:D:96:MET:CE	1:D:101:ILE:HG12	2.51	0.41
1:C:319:PRO:HA	1:C:320:PRO:HD3	1.97	0.41
1:F:171:ALA:C	1:F:173:TRP:H	2.24	0.41
1:D:468:LEU:O	1:D:472:ILE:HG13	2.21	0.41
1:B:351:LEU:O	1:B:351:LEU:HD12	2.20	0.41
1:F:98:ILE:HG21	1:F:132:VAL:CG2	2.51	0.41
1:A:8:PHE:HD1	1:A:71:PRO:HG2	1.86	0.41
1:C:342:VAL:HG23	1:C:343:GLY:N	2.33	0.41
1:D:347:THR:HG21	1:E:298:GLU:OE1	2.20	0.41
1:D:98:ILE:HD11	1:D:113:TRP:CD1	2.56	0.41
1:B:404:ILE:HA	1:B:442:VAL:HG13	2.01	0.41
1:A:98:ILE:HD11	1:A:113:TRP:CE2	2.55	0.41
1:B:265:PRO:O	1:B:288:SER:HB3	2.20	0.41
1:E:369:ASN:O	1:E:370:SER:C	2.59	0.41
1:A:499:ALA:HB1	1:A:520:ALA:HB3	2.02	0.41
1:F:272:ASN:HD22	1:F:272:ASN:HA	1.51	0.41
1:E:342:VAL:HG23	1:E:343:GLY:N	2.34	0.41
1:E:367:LYS:NZ	1:E:466:CYS:HA	2.35	0.41
1:C:278:PHE:CE2	1:C:467:SER:OG	2.70	0.41
1:B:189:ARG:HG3	1:B:193:GLN:NE2	2.36	0.41
1:A:495:LEU:HD22	1:A:521:LEU:HD22	2.02	0.41
1:F:282:VAL:HG21	1:F:467:SER:OG	2.19	0.41
1:B:427:ILE:C	1:B:429:GLY:N	2.74	0.41
1:D:124:LEU:HD11	1:D:174:CYS:SG	2.61	0.41
1:D:266:LEU:HD11	1:D:291:ILE:HG13	2.01	0.41
1:C:357:LEU:HA	1:C:360:PHE:CD1	2.56	0.41
1:C:182:LEU:HD12	1:C:190:VAL:HG21	2.03	0.41
1:C:329:ALA:O	1:C:333:VAL:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:117:PHE:HA	1:F:118:PRO:HD3	1.91	0.41
1:B:196:SER:HB3	1:B:201:ARG:H	1.86	0.41
1:E:249:THR:HG23	1:E:252:GLU:OE1	2.21	0.41
1:E:358:LEU:HD22	1:E:409:TYR:CD2	2.55	0.41
1:A:270:ILE:HD12	1:A:310:LEU:HD11	2.03	0.41
1:F:283:THR:CG2	1:F:288:SER:HB2	2.51	0.41
1:C:402:THR:O	1:C:403:LYS:C	2.60	0.41
1:E:402:THR:OG1	1:E:415:CYS:HB2	2.21	0.41
1:C:192:TYR:CZ	1:C:410:LYS:HB3	2.56	0.41
1:E:167:GLU:C	1:E:169:ASN:N	2.74	0.41
1:A:55:ILE:CG1	1:A:80:VAL:HG13	2.52	0.40
1:E:299:VAL:HG21	1:E:326:ALA:CA	2.38	0.40
1:D:313:ASN:O	1:D:314:THR:C	2.60	0.40
1:B:160:ILE:HD11	1:B:193:GLN:O	2.20	0.40
1:E:349:THR:HG21	1:F:297:SER:OG	2.21	0.40
1:F:66:HIS:HE1	1:F:87:ASP:OD1	2.04	0.40
1:D:437:THR:O	1:D:438:ASN:C	2.59	0.40
1:E:276:GLN:CG	1:E:292:MET:HE2	2.51	0.40
1:D:21:ILE:HD11	1:D:27:LEU:CD1	2.50	0.40
1:C:75:ASN:ND2	1:C:76:ASP:OD1	2.54	0.40
1:B:167:GLU:C	1:B:169:ASN:N	2.72	0.40
1:B:70:VAL:HA	1:B:71:PRO:HD3	1.82	0.40
1:B:296:GLN:HG3	1:B:322:MET:HB2	2.03	0.40
1:A:14:LEU:HB3	1:A:42:VAL:HG22	2.03	0.40
1:C:495:LEU:HD22	1:C:495:LEU:O	2.20	0.40
1:D:189:ARG:O	1:D:193:GLN:HG2	2.20	0.40
2:E:541:3NM:N	3:E:542:IFP:C7A	2.85	0.40
1:B:228:LEU:N	1:B:228:LEU:CD1	2.85	0.40
1:F:356:LEU:O	1:F:357:LEU:C	2.60	0.40
1:D:427:ILE:HG22	1:D:427:ILE:O	2.21	0.40
1:D:143:THR:HG23	1:D:143:THR:O	2.22	0.40
1:F:77:ARG:HE	1:F:80:VAL:CG2	2.35	0.40
1:E:276:GLN:HG3	1:E:292:MET:HE2	2.03	0.40
1:E:269:HIS:HB2	1:E:292:MET:SD	2.61	0.40
1:B:189:ARG:HG3	1:B:193:GLN:HE21	1.86	0.40
1:B:192:TYR:HA	1:B:431:TYR:HB3	2.04	0.40
1:B:145:THR:O	1:B:145:THR:HG22	2.20	0.40
1:A:121:VAL:O	1:A:124:LEU:HB3	2.21	0.40
1:B:165:ALA:O	1:B:169:ASN:HB2	2.21	0.40
1:B:344:TYR:CZ	1:B:376:LEU:HD23	2.57	0.40
1:A:218:ALA:O	1:A:219:ALA:C	2.60	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:LEU:HA	1:B:163:LEU:HD23	1.89	0.40
1:F:312:LEU:HD13	1:F:312:LEU:HA	1.91	0.40
1:E:274:VAL:HG12	1:F:277:ASN:HA	2.04	0.40
1:A:192:TYR:C	1:A:192:TYR:CD2	2.92	0.40
1:A:192:TYR:CD2	1:A:192:TYR:O	2.75	0.40
1:B:276:GLN:CG	1:B:292:MET:HG3	2.51	0.40
1:A:529:THR:N	1:A:530:PRO:HD3	2.36	0.40
1:E:339:PHE:HE1	1:E:357:LEU:HD23	1.85	0.40
1:C:310:LEU:HD21	1:C:312:LEU:HD21	2.03	0.40
1:A:94:ASP:O	1:E:52:LYS:HB2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	493/540 (91%)	398 (81%)	78 (16%)	17 (3%)	5	31
1	B	493/540 (91%)	423 (86%)	49 (10%)	21 (4%)	3	25
1	C	493/540 (91%)	430 (87%)	42 (8%)	21 (4%)	3	25
1	D	493/540 (91%)	411 (83%)	61 (12%)	21 (4%)	3	25
1	E	489/540 (91%)	418 (86%)	49 (10%)	22 (4%)	3	24
1	F	493/540 (91%)	411 (83%)	70 (14%)	12 (2%)	7	43
All	All	2954/3240 (91%)	2491 (84%)	349 (12%)	114 (4%)	4	28

All (114) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	20	MET
1	A	76	ASP

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Mol	Chain	Res	Type
1	A	247	LEU
1	A	317	VAL
1	B	20	MET
1	B	126	LYS
1	B	317	VAL
1	C	76	ASP
1	C	247	LEU
1	C	314	THR
1	C	438	ASN
1	C	481	SER
1	D	20	MET
1	D	76	ASP
1	D	138	GLY
1	D	247	LEU
1	D	314	THR
1	D	342	VAL
1	D	344	TYR
1	D	370	SER
1	D	438	ASN
1	D	528	ASN
1	E	20	MET
1	E	76	ASP
1	E	272	ASN
1	E	317	VAL
1	F	20	MET
1	F	76	ASP
1	F	126	LYS
1	F	247	LEU
1	F	272	ASN
1	F	317	VAL
1	F	438	ASN
1	A	138	GLY
1	A	168	ARG
1	A	438	ASN
1	A	441	SER
1	A	528	ASN
1	B	11	SER
1	B	138	GLY
1	B	247	LEU
1	B	370	SER
1	B	439	GLY
1	C	20	MET

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Mol	Chain	Res	Type
1	C	138	GLY
1	C	172	HIS
1	C	238	ASN
1	C	317	VAL
1	D	11	SER
1	D	343	GLY
1	E	126	LYS
1	E	138	GLY
1	E	247	LEU
1	E	342	VAL
1	E	343	GLY
1	E	344	TYR
1	F	172	HIS
1	A	152	ALA
1	A	345	SER
1	A	481	SER
1	B	76	ASP
1	B	172	HIS
1	B	272	ASN
1	B	315	GLY
1	B	481	SER
1	C	49	ALA
1	C	272	ASN
1	C	345	SER
1	C	370	SER
1	C	410	LYS
1	D	152	ALA
1	D	186	ASN
1	D	395	ASN
1	D	442	VAL
1	D	452	ALA
1	D	481	SER
1	E	345	SER
1	F	314	THR
1	F	410	LYS
1	B	344	TYR
1	C	170	ASN
1	C	495	LEU
1	D	217	ASP
1	E	6	GLU
1	E	170	ASN
1	E	438	ASN

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Mol	Chain	Res	Type
1	F	11	SER
1	F	276	GLN
1	A	272	ASN
1	A	314	THR
1	B	343	GLY
1	B	428	GLU
1	C	254	GLN
1	C	344	TYR
1	E	186	ASN
1	E	494	MET
1	E	495	LEU
1	E	535	PRO
1	A	170	ASN
1	B	186	ASN
1	B	238	ASN
1	B	438	ASN
1	C	105	VAL
1	E	370	SER
1	B	97	PRO
1	B	483	GLY
1	E	315	GLY
1	A	343	GLY
1	C	343	GLY
1	E	97	PRO
1	A	448	VAL
1	D	148	ASN
1	E	105	VAL
1	D	317	VAL

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	405/449 (90%)	361 (89%)	44 (11%)	8 33
1	B	405/449 (90%)	352 (87%)	53 (13%)	5 24
1	C	405/449 (90%)	346 (85%)	59 (15%)	4 18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	405/449 (90%)	358 (88%)	47 (12%)	7 30
1	E	403/449 (90%)	352 (87%)	51 (13%)	5 25
1	F	405/449 (90%)	352 (87%)	53 (13%)	5 24
All	All	2428/2694 (90%)	2121 (87%)	307 (13%)	5 26

All (307) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LYS
1	A	13	TYR
1	A	16	THR
1	A	54	PHE
1	A	64	LEU
1	A	70	VAL
1	A	78	ILE
1	A	94	ASP
1	A	98	ILE
1	A	105	VAL
1	A	113	TRP
1	A	117	PHE
1	A	139	THR
1	A	140	LEU
1	A	144	LEU
1	A	160	ILE
1	A	177	VAL
1	A	185	ASP
1	A	187	ILE
1	A	191	LEU
1	A	192	TYR
1	A	216	LEU
1	A	226	ARG
1	A	228	LEU
1	A	242	SER
1	A	260	THR
1	A	272	ASN
1	A	296	GLN
1	A	311	LEU
1	A	312	LEU
1	A	317	VAL
1	A	322	MET
1	A	328	ARG

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Mol	Chain	Res	Type
1	A	335	ARG
1	A	337	ILE
1	A	352	LEU
1	A	362	GLN
1	A	374	LEU
1	A	437	THR
1	A	467	SER
1	A	481	SER
1	A	482	GLU
1	A	495	LEU
1	A	524	LEU
1	B	2	LYS
1	B	4	SER
1	B	13	TYR
1	B	51	THR
1	B	54	PHE
1	B	78	ILE
1	B	82	MET
1	B	93	GLN
1	B	104	LEU
1	B	105	VAL
1	B	113	TRP
1	B	124	LEU
1	B	140	LEU
1	B	144	LEU
1	B	182	LEU
1	B	187	ILE
1	B	191	LEU
1	B	197	SER
1	B	202	SER
1	B	221	SER
1	B	226	ARG
1	B	241	LEU
1	B	260	THR
1	B	266	LEU
1	B	272	ASN
1	B	275	HIS
1	B	284	LEU
1	B	291	ILE
1	B	292	MET
1	B	293	SER
1	B	296	GLN

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Mol	Chain	Res	Type
1	B	297	SER
1	B	302	LEU
1	B	312	LEU
1	B	322	MET
1	B	328	ARG
1	B	333	VAL
1	B	337	ILE
1	B	342	VAL
1	B	350	ARG
1	B	352	LEU
1	B	371	SER
1	B	372	GLU
1	B	399	ILE
1	B	418	GLU
1	B	428	GLU
1	B	443	GLU
1	B	481	SER
1	B	482	GLU
1	B	495	LEU
1	B	510	SER
1	B	515	VAL
1	B	517	LEU
1	C	2	LYS
1	C	11	SER
1	C	13	TYR
1	C	54	PHE
1	C	64	LEU
1	C	70	VAL
1	C	78	ILE
1	C	82	MET
1	C	89	ILE
1	C	105	VAL
1	C	113	TRP
1	C	124	LEU
1	C	144	LEU
1	C	161	ARG
1	C	182	LEU
1	C	185	ASP
1	C	191	LEU
1	C	193	GLN
1	C	195	VAL
1	C	207	CYS

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Mol	Chain	Res	Type
1	C	208	VAL
1	C	221	SER
1	C	226	ARG
1	C	228	LEU
1	C	241	LEU
1	C	249	THR
1	C	266	LEU
1	C	272	ASN
1	C	274	VAL
1	C	275	HIS
1	C	284	LEU
1	C	289	SER
1	C	291	ILE
1	C	293	SER
1	C	296	GLN
1	C	297	SER
1	C	302	LEU
1	C	311	LEU
1	C	312	LEU
1	C	322	MET
1	C	328	ARG
1	C	337	ILE
1	C	348	GLU
1	C	352	LEU
1	C	371	SER
1	C	374	LEU
1	C	399	ILE
1	C	404	ILE
1	C	443	GLU
1	C	466	CYS
1	C	467	SER
1	C	481	SER
1	C	482	GLU
1	C	495	LEU
1	C	510	SER
1	C	515	VAL
1	C	517	LEU
1	C	524	LEU
1	C	538	THR
1	D	2	LYS
1	D	13	TYR
1	D	16	THR

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Mol	Chain	Res	Type
1	D	54	PHE
1	D	64	LEU
1	D	75	ASN
1	D	76	ASP
1	D	77	ARG
1	D	78	ILE
1	D	124	LEU
1	D	139	THR
1	D	144	LEU
1	D	177	VAL
1	D	182	LEU
1	D	186	ASN
1	D	191	LEU
1	D	192	TYR
1	D	196	SER
1	D	216	LEU
1	D	241	LEU
1	D	250	THR
1	D	260	THR
1	D	272	ASN
1	D	284	LEU
1	D	291	ILE
1	D	293	SER
1	D	297	SER
1	D	302	LEU
1	D	312	LEU
1	D	313	ASN
1	D	314	THR
1	D	322	MET
1	D	328	ARG
1	D	335	ARG
1	D	348	GLU
1	D	350	ARG
1	D	352	LEU
1	D	362	GLN
1	D	372	GLU
1	D	374	LEU
1	D	416	THR
1	D	467	SER
1	D	482	GLU
1	D	495	LEU
1	D	504	SER

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Mol	Chain	Res	Type
1	D	519	ASP
1	D	524	LEU
1	E	4	SER
1	E	13	TYR
1	E	40	THR
1	E	54	PHE
1	E	63	GLU
1	E	64	LEU
1	E	77	ARG
1	E	78	ILE
1	E	94	ASP
1	E	101	ILE
1	E	113	TRP
1	E	134	TYR
1	E	143	THR
1	E	144	LEU
1	E	154	MET
1	E	156	THR
1	E	160	ILE
1	E	177	VAL
1	E	186	ASN
1	E	189	ARG
1	E	191	LEU
1	E	193	GLN
1	E	197	SER
1	E	226	ARG
1	E	241	LEU
1	E	249	THR
1	E	257	ILE
1	E	271	THR
1	E	284	LEU
1	E	289	SER
1	E	296	GLN
1	E	297	SER
1	E	311	LEU
1	E	312	LEU
1	E	313	ASN
1	E	322	MET
1	E	328	ARG
1	E	348	GLU
1	E	349	THR
1	E	352	LEU

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Mol	Chain	Res	Type
1	E	362	GLN
1	E	399	ILE
1	E	442	VAL
1	E	446	PRO
1	E	466	CYS
1	E	467	SER
1	E	495	LEU
1	E	504	SER
1	E	515	VAL
1	E	524	LEU
1	E	532	THR
1	F	2	LYS
1	F	13	TYR
1	F	16	THR
1	F	40	THR
1	F	54	PHE
1	F	61	ILE
1	F	64	LEU
1	F	70	VAL
1	F	76	ASP
1	F	78	ILE
1	F	82	MET
1	F	89	ILE
1	F	91	VAL
1	F	94	ASP
1	F	105	VAL
1	F	113	TRP
1	F	124	LEU
1	F	139	THR
1	F	144	LEU
1	F	161	ARG
1	F	187	ILE
1	F	191	LEU
1	F	226	ARG
1	F	241	LEU
1	F	272	ASN
1	F	274	VAL
1	F	276	GLN
1	F	284	LEU
1	F	289	SER
1	F	291	ILE
1	F	296	GLN

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Mol	Chain	Res	Type
1	F	297	SER
1	F	299	VAL
1	F	300	ASN
1	F	302	LEU
1	F	311	LEU
1	F	322	MET
1	F	328	ARG
1	F	333	VAL
1	F	342	VAL
1	F	357	LEU
1	F	362	GLN
1	F	374	LEU
1	F	408	LYS
1	F	415	CYS
1	F	418	GLU
1	F	466	CYS
1	F	482	GLU
1	F	495	LEU
1	F	514	GLN
1	F	524	LEU
1	F	532	THR
1	F	538	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (62) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	HIS
1	A	93	GLN
1	A	169	ASN
1	A	183	HIS
1	A	193	GLN
1	A	281	ASN
1	A	313	ASN
1	A	479	GLN
1	A	484	ASN
1	B	37	ASN
1	B	66	HIS
1	B	169	ASN
1	B	172	HIS
1	B	183	HIS
1	B	193	GLN
1	B	269	HIS

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Mol	Chain	Res	Type
1	B	272	ASN
1	B	281	ASN
1	B	484	ASN
1	C	43	GLN
1	C	75	ASN
1	C	93	GLN
1	C	169	ASN
1	C	193	GLN
1	C	272	ASN
1	C	355	ASN
1	C	484	ASN
1	D	75	ASN
1	D	93	GLN
1	D	169	ASN
1	D	186	ASN
1	D	193	GLN
1	D	259	ASN
1	D	272	ASN
1	D	275	HIS
1	D	276	GLN
1	D	281	ASN
1	D	313	ASN
1	D	355	ASN
1	D	484	ASN
1	E	43	GLN
1	E	66	HIS
1	E	93	GLN
1	E	186	ASN
1	E	275	HIS
1	E	281	ASN
1	E	313	ASN
1	E	355	ASN
1	E	362	GLN
1	E	484	ASN
1	F	43	GLN
1	F	66	HIS
1	F	93	GLN
1	F	169	ASN
1	F	193	GLN
1	F	259	ASN
1	F	272	ASN
1	F	313	ASN

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Mol	Chain	Res	Type
1	F	355	ASN
1	F	479	GLN
1	F	484	ASN
1	F	514	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 24 ligands modelled in this entry, 6 are monoatomic - leaving 18 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	3NM	A	541	-	11,16,16	5.51	5 (45%)	9,23,23	2.81	2 (22%)
3	IFP	A	542	-	5,12,12	7.11	4 (80%)	3,18,18	2.48	1 (33%)
4	POP	A	543	5	8,8,8	0.48	0	13,13,13	1.36	1 (7%)
2	3NM	B	541	-	11,16,16	5.53	4 (36%)	9,23,23	2.58	2 (22%)
3	IFP	B	542	-	5,12,12	7.35	4 (80%)	3,18,18	2.31	1 (33%)
4	POP	B	543	5	8,8,8	0.63	0	13,13,13	1.52	1 (7%)
2	3NM	C	541	-	11,16,16	5.58	4 (36%)	9,23,23	2.15	2 (22%)
3	IFP	C	542	-	5,12,12	7.21	4 (80%)	3,18,18	2.35	1 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	POP	C	543	5	8,8,8	0.52	0	13,13,13	1.37	1 (7%)
2	3NM	D	541	-	11,16,16	5.56	4 (36%)	9,23,23	2.61	2 (22%)
3	IFP	D	542	-	5,12,12	7.05	4 (80%)	3,18,18	2.42	1 (33%)
4	POP	D	543	5	8,8,8	0.61	0	13,13,13	1.31	1 (7%)
2	3NM	E	541	-	11,16,16	5.60	4 (36%)	9,23,23	2.37	2 (22%)
3	IFP	E	542	-	5,12,12	7.18	4 (80%)	3,18,18	2.30	1 (33%)
4	POP	E	543	5	8,8,8	0.49	0	13,13,13	1.44	1 (7%)
2	3NM	F	541	-	11,16,16	5.42	4 (36%)	9,23,23	3.88	2 (22%)
3	IFP	F	542	-	5,12,12	7.18	4 (80%)	3,18,18	2.40	1 (33%)
4	POP	F	543	5	8,8,8	0.52	0	13,13,13	1.41	1 (7%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	3NM	A	541	-	-	0/6/11/11	0/1/1/1
3	IFP	A	542	-	-	0/0/19/19	0/1/1/1
4	POP	A	543	5	-	0/6/6/6	0/0/0/0
2	3NM	B	541	-	-	0/6/11/11	0/1/1/1
3	IFP	B	542	-	-	0/0/19/19	0/1/1/1
4	POP	B	543	5	-	0/6/6/6	0/0/0/0
2	3NM	C	541	-	-	0/6/11/11	0/1/1/1
3	IFP	C	542	-	-	0/0/19/19	0/1/1/1
4	POP	C	543	5	-	0/6/6/6	0/0/0/0
2	3NM	D	541	-	-	0/6/11/11	0/1/1/1
3	IFP	D	542	-	-	0/0/19/19	0/1/1/1
4	POP	D	543	5	-	0/6/6/6	0/0/0/0
2	3NM	E	541	-	-	0/6/11/11	0/1/1/1
3	IFP	E	542	-	-	0/0/19/19	0/1/1/1
4	POP	E	543	5	-	0/6/6/6	0/0/0/0
2	3NM	F	541	-	-	0/6/11/11	0/1/1/1
3	IFP	F	542	-	-	0/0/19/19	0/1/1/1
4	POP	F	543	5	-	0/6/6/6	0/0/0/0

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	541	3NM	C5-S	-12.91	1.50	1.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	541	3NM	C5-S	-12.90	1.50	1.74
2	B	541	3NM	C5-S	-12.87	1.50	1.74
2	C	541	3NM	C5-S	-12.65	1.50	1.74
2	A	541	3NM	C5-S	-12.48	1.50	1.74
2	F	541	3NM	C5-S	-12.30	1.51	1.74
2	B	541	3NM	C3-S	-3.28	1.69	1.73
2	A	541	3NM	C3-S	-3.25	1.69	1.73
2	F	541	3NM	C3-S	-3.23	1.69	1.73
2	D	541	3NM	C3-S	-3.19	1.69	1.73
2	E	541	3NM	C3-S	-3.10	1.69	1.73
3	E	542	IFP	C5A-C4A	-3.05	1.37	1.43
3	C	542	IFP	C5A-C4A	-3.04	1.37	1.43
3	D	542	IFP	C5A-C4A	-2.98	1.37	1.43
3	F	542	IFP	C5A-C4A	-2.91	1.38	1.43
2	C	541	3NM	C3-S	-2.89	1.69	1.73
3	B	542	IFP	C5A-C4A	-2.87	1.38	1.43
3	A	542	IFP	C5A-C4A	-2.54	1.38	1.43
2	A	541	3NM	O3-C7	-2.08	1.36	1.44
3	F	542	IFP	C6A-N1A	3.93	1.40	1.32
3	A	542	IFP	C6A-N1A	3.95	1.40	1.32
3	D	542	IFP	C6A-N1A	4.00	1.40	1.32
3	B	542	IFP	C6A-N1A	4.28	1.40	1.32
3	C	542	IFP	C6A-N1A	4.31	1.41	1.32
3	E	542	IFP	C6A-N1A	4.52	1.41	1.32
3	D	542	IFP	C4A-N4A	7.52	1.42	1.29
3	E	542	IFP	C4A-N4A	7.56	1.42	1.29
3	A	542	IFP	C4A-N4A	7.57	1.42	1.29
2	F	541	3NM	C5-C2	7.81	1.58	1.42
3	F	542	IFP	C4A-N4A	7.82	1.43	1.29
2	A	541	3NM	C5-C2	7.89	1.58	1.42
2	D	541	3NM	C5-C2	7.96	1.58	1.42
2	B	541	3NM	C5-C2	7.96	1.58	1.42
2	C	541	3NM	C5-C2	8.00	1.58	1.42
3	C	542	IFP	C4A-N4A	8.07	1.43	1.29
3	B	542	IFP	C4A-N4A	8.08	1.43	1.29
2	E	541	3NM	C5-C2	8.13	1.58	1.42
2	B	541	3NM	C3-N	9.23	1.44	1.31
2	F	541	3NM	C3-N	9.41	1.45	1.31
2	D	541	3NM	C3-N	9.53	1.45	1.31
2	A	541	3NM	C3-N	9.65	1.45	1.31
2	E	541	3NM	C3-N	9.68	1.45	1.31
2	C	541	3NM	C3-N	9.97	1.45	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	542	IFP	C7A-C5A	12.92	1.49	1.33
3	C	542	IFP	C7A-C5A	12.94	1.49	1.33
3	E	542	IFP	C7A-C5A	13.08	1.49	1.33
3	F	542	IFP	C7A-C5A	13.14	1.49	1.33
3	A	542	IFP	C7A-C5A	13.16	1.49	1.33
3	B	542	IFP	C7A-C5A	13.35	1.50	1.33

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	541	3NM	C6-C5-C2	-8.23	120.19	127.56
2	A	541	3NM	C6-C5-C2	-5.16	122.94	127.56
4	B	543	POP	P2-O-P1	-4.65	119.66	132.73
4	E	543	POP	P2-O-P1	-4.58	119.88	132.73
2	B	541	3NM	C6-C5-C2	-4.56	123.48	127.56
4	F	543	POP	P2-O-P1	-4.17	121.01	132.73
2	D	541	3NM	C6-C5-C2	-3.99	123.99	127.56
4	A	543	POP	P2-O-P1	-3.91	121.76	132.73
4	D	543	POP	P2-O-P1	-3.88	121.83	132.73
3	A	542	IFP	C5A-C6A-N1A	-3.85	119.97	125.38
4	C	543	POP	P2-O-P1	-3.71	122.30	132.73
3	D	542	IFP	C5A-C6A-N1A	-3.62	120.29	125.38
3	F	542	IFP	C5A-C6A-N1A	-3.60	120.32	125.38
2	E	541	3NM	C6-C5-C2	-3.50	124.43	127.56
2	C	541	3NM	C6-C5-C2	-3.23	124.67	127.56
3	C	542	IFP	C5A-C6A-N1A	-3.21	120.87	125.38
3	B	542	IFP	C5A-C6A-N1A	-3.21	120.87	125.38
3	E	542	IFP	C5A-C6A-N1A	-3.09	121.04	125.38
2	C	541	3NM	C6-C5-S	5.09	127.36	120.24
2	E	541	3NM	C6-C5-S	5.75	128.29	120.24
2	B	541	3NM	C6-C5-S	5.95	128.56	120.24
2	D	541	3NM	C6-C5-S	6.46	129.28	120.24
2	A	541	3NM	C6-C5-S	6.47	129.29	120.24
2	F	541	3NM	C6-C5-S	7.88	131.26	120.24

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	541	3NM	3	0
3	A	542	IFP	1	0
4	A	543	POP	1	0
2	B	541	3NM	3	0
3	B	542	IFP	1	0
4	B	543	POP	2	0
2	D	541	3NM	1	0
2	E	541	3NM	2	0
3	E	542	IFP	2	0
2	F	541	3NM	2	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	507/540 (93%)	-0.39	2 (0%) 93 90	30, 79, 99, 120	0
1	B	507/540 (93%)	-0.41	0 100 100	41, 81, 103, 127	0
1	C	507/540 (93%)	-0.34	3 (0%) 90 85	41, 74, 96, 117	0
1	D	507/540 (93%)	-0.37	2 (0%) 93 90	39, 75, 99, 120	0
1	E	505/540 (93%)	-0.42	1 (0%) 95 94	42, 80, 101, 124	0
1	F	507/540 (93%)	-0.40	2 (0%) 93 90	42, 78, 100, 119	0
All	All	3040/3240 (93%)	-0.39	10 (0%) 94 93	30, 78, 101, 127	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	465	GLY	4.6
1	E	437	THR	3.0
1	A	465	GLY	2.7
1	F	275	HIS	2.4
1	D	540	THR	2.3
1	A	277	ASN	2.3
1	C	277	ASN	2.2
1	D	277	ASN	2.2
1	C	281	ASN	2.1
1	C	279	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	MG	A	544	1/1	0.97	0.33	5.92	66,66,66,66	0
5	MG	E	544	1/1	0.88	0.28	3.66	61,61,61,61	0
5	MG	D	544	1/1	0.92	0.27	2.36	61,61,61,61	0
4	POP	D	543	9/9	0.97	0.22	1.61	61,72,74,74	0
3	IFP	E	542	12/12	0.97	0.22	1.55	68,73,80,80	0
4	POP	B	543	9/9	0.97	0.22	1.26	70,78,81,87	0
4	POP	A	543	9/9	0.98	0.20	1.00	64,80,89,91	0
2	3NM	B	541	16/16	0.94	0.21	1.00	76,78,85,88	0
4	POP	F	543	9/9	0.97	0.21	0.86	68,79,86,86	0
2	3NM	D	541	16/16	0.96	0.21	0.79	70,75,81,83	0
4	POP	E	543	9/9	0.97	0.19	0.58	64,79,88,90	0
3	IFP	B	542	12/12	0.96	0.19	0.58	75,77,81,83	0
4	POP	C	543	9/9	0.99	0.17	0.49	62,72,80,82	0
3	IFP	D	542	12/12	0.98	0.18	0.44	65,69,72,74	0
2	3NM	A	541	16/16	0.97	0.18	0.39	71,77,84,87	0
3	IFP	A	542	12/12	0.97	0.18	0.33	70,73,77,77	0
2	3NM	E	541	16/16	0.96	0.17	-0.06	69,76,79,83	0
2	3NM	F	541	16/16	0.97	0.17	-0.26	69,78,87,88	0
3	IFP	C	542	12/12	0.98	0.16	-0.34	62,66,71,74	0
3	IFP	F	542	12/12	0.98	0.16	-0.36	70,74,78,79	0
2	3NM	C	541	16/16	0.98	0.15	-0.82	65,69,75,77	0
5	MG	C	544	1/1	0.94	0.30	-	56,56,56,56	0
5	MG	F	544	1/1	0.91	0.33	-	60,60,60,60	0
5	MG	B	544	1/1	0.90	0.32	-	56,56,56,56	0

6.5 Other polymers (i)

There are no such residues in this entry.